

6  
Access DB# 716721  
**SEARCH REQUEST FORM**

Scientific and Technical Information Center

Requester's Full Name: HARVEY Examiner #: 71136 Date: 9/30/02  
Art Unit: 1751 Phone Number 305-559 Serial Number: 091954772  
Mail Box and Bldg/Room Location: 5B36 Results Format Preferred (circle): PAPER DISK E-MAIL

**If more than one search is submitted, please prioritize searches in order of need.**

\*\*\*\*\*  
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: \_\_\_\_\_

Inventors (please provide full names): \_\_\_\_\_

Earliest Priority Filing Date: \_\_\_\_\_

*\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Anything you can find on the  
highlighted compounds.

Thanks

**STAFF USE ONLY**

Searcher: 22  
Searcher Phone #: \_\_\_\_\_  
Searcher Location: \_\_\_\_\_  
Date Searcher Picked Up: \_\_\_\_\_  
Date Completed: 10-1-02  
Searcher Prep & Review Time: 5  
Clerical Prep Time: \_\_\_\_\_  
Online Time: 65

**Type of Search**

NA Sequence (#) \_\_\_\_\_  
AA Sequence (#) \_\_\_\_\_  
Structure (#) (6)  
Bibliographic \_\_\_\_\_  
Litigation \_\_\_\_\_  
Fulltext \_\_\_\_\_  
Patent Family \_\_\_\_\_  
Other \_\_\_\_\_

**Vendors and cost where applicable**

STN # 319.10  
Dialog \_\_\_\_\_  
Questel/Orbit \_\_\_\_\_  
Dr.Link \_\_\_\_\_  
Lexis/Nexis \_\_\_\_\_  
Sequence Systems \_\_\_\_\_  
WWW/Internet \_\_\_\_\_  
Other (specify) \_\_\_\_\_

# EIC1700

## Search Results

### Feedback Form (Optional)



Scientific & Technical Information Center

The search results generated for your recent request are attached. If you have any questions or comments (compliments or complaints) about the scope or the results of the search, please contact *the EIC searcher* who conducted the search *or contact*:

Kathleen Fuller, Team Leader, 308-4290, CP3/4 3D62

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#### Voluntary Results Feedback Form

➤ I am an examiner in Workgroup:  Example:

➤ Relevant prior art *found*, search results used as follows:

- ☐ 102 rejection
- ☐ 103 rejection
- ☐ Cited as being of interest.
- ☐ Helped examiner better understand the invention.
- ☐ Helped examiner better understand the state of the art in their technology.

*Types of relevant prior art found:*

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature  
(journal articles, conference proceedings, new product announcements etc.)

➤ Relevant prior art *not found*:

- ☐ Results verified the lack of relevant prior art (helped determine patentability).
- ☐ Search results were not useful in determining patentability or understanding the invention.

**Other Comments:**

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Drop off completed forms in CP3/4 - 3D62 .

I hereby certify that this paper/fee is being deposited with the United States Postal Service "Express Mail Post Office to Addressee" service under 37 CFR 1.10 on the date indicated above and is addressed to the Assistant Commissioner For Patents, Washington, D.C. 20231.

Frank C. Turner 39,863  
 Attorney mailing application Reg No.  
*Frank C. Turner*  
 Signature of Attorney mailing application

Case 6009RXD

## IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re application of Trinh, et al. ::  
 Serial No. :: Group Art Unit: 1755  
 Filed :: Examiner: A. Green  
 Confirmation No. ::  
 For CONCENTRATED, STABLE  
 FABRIC SOFTENING  
 COMPOSITION

PRELIMINARY AMENDMENT

Commissioner for Patents  
 Washington, D.C. 20231

Dear Sir:

Before computing the fees for entering the captioned Divisional Application, please enter the following amendment.

IN THE SPECIFICATION

Page 1, line 15, please insert -

~~This is a Divisional Patent Application of Patent Application Serial No.~~  
 08/983,542, filed September 25, 1998, which is ~~pending~~ -

now US 6,323,172.

IN THE CLAIMS

Please cancel claims 1-123 without prejudice.

Please add new claims 124-145 as follows.

124. Principal solvent selected from the group consisting of:

JAH  
11/1/02

A. compound selected from the group consisting of 1,2-butanediol, 2,3,3-trimethyl-

→ 3,4-pentanediol, 2,3-dimethyl-, 2,3-hexanediol, 4-methyl-, 2,3-hexanediol, 5-

Sam → methyl-, 3,4-hexanediol, 2-methyl-, 1,2-butanediol, 2,3,3-trimethyl-, 3,4-

pentanediol, 2,3-dimethyl-, 1,3-propanediol, 2-(1,1-dimethylpropyl)-, 1,3-

propanediol, 2-(1,2-dimethylpropyl)-, 1,3-propanediol, 2-(2,2-dimethylpropyl)-,

1,3-butanediol, 2-(1-methylpropyl)-, 1,3-butanediol, 2-ethyl-2,3-dimethyl-, 1,3-

butanediol, 2-(2-methylpropyl)-, 1,3-butanediol, 2-methyl-2-isopropyl-, 1,3-

butanediol, 3-methyl-2-isopropyl-, 1,3-butanediol, 3-methyl-2-propyl-, 1,4-

butanediol, 2,2-diethyl-, 1,4-butanediol, 2-methyl-2-propyl-, 1,4-butanediol, 2-(1-

methylpropyl)-, 1,4-butanediol, 2-ethyl-2,3-dimethyl-, 1,4-butanediol, 2-ethyl-3,3-

dimethyl-, 1,4-butanediol, 2-(2-methylpropyl)-, 1,4-pentanediol, 2,2,3-trimethyl-,

1,4-pentanediol, 2,3,3-trimethyl-, 1,5-pentanediol, 2,2,3-trimethyl-, 1,5-

pentanediol, 2,3,3-trimethyl-, 1,3-pentanediol, 2-ethyl-2-methyl-, 1,4-pentanediol,

2-ethyl-2-methyl-, 1,4-pentanediol, 2-ethyl-3-methyl-, 1,4-pentanediol, 2-ethyl-4-

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1,5-pentanediol, 2-ethyl-2-methyl-, 1,5-pentanediol, 2-ethyl-4-methyl-, 2,4-

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propyl-, 1,4-pentanediol, 2-isopropyl-, 1,4-pentanediol, 2-propyl-, 1,4-pentanediol,

3-isopropyl-, 2,4-pentanediol, 3-propyl-, 1,3-hexanediol, 2,3-dimethyl-, 1,3-

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3-ethyl-, 2,5-hexanediol, 3-ethyl-, 1,3-heptanediol, 4-methyl-, 1,3-heptanediol, 5-

methyl-, 1,3-heptanediol, 6-methyl-, 1,5-heptanediol, 3-methyl-, 1,5-heptanediol,

4-methyl-, 1,6-heptanediol, 3-methyl-, 1,6-heptanediol, 5-methyl-, 2,4-

heptanediol, 5-methyl-, 2,5-heptanediol, 3-methyl-, 3,5-heptanediol, 2-methyl-,

2,6-octanediol, 2,4-hexanediol, 3,3,4-trimethyl-, 2,4-hexanediol, 3,5,5-trimethyl-,

2,4-hexanediol, 4,5,5-trimethyl-, 2,5-hexanediol, 3,3,4-trimethyl-, 2,5-hexanediol,

3,3,5-trimethyl-,

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DICTIONARY FILE UPDATES: 29 SEP 2002 HIGHEST RN 457047-85-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when  
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP  
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in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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L1 STR  
L2 STR  
L3 STR  
L4 STR  
L5 STR  
L6 STR

FILE 'REGISTRY' ENTERED AT 13:27:32 ON 01 OCT 2002

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L8 3 S L1 FAM FUL  
L9 0 S L2 FAM  
SAV L8 HAR772A/A  
L10 11 S L2 FAM FUL  
SAV L10 HAR772B/A  
L11 0 S L3 FAM  
L12 1 S L3 FAM FUL  
SAV L10 HAR772C/A  
L13 0 S L4 FAM  
L14 1 S L4 FAM FUL  
DEL HAR772C/A  
SAV L12 HAR772C/A  
SAV L14 HAR772D/A

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L18      3 S L6 FAM FUL
          SAV L18 HAR772F/A

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L20      0 S L10
L21      0 S L12
L22      0 S L14
L23      3 S L16
L24      0 S L18

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FILE 'ZCAPLUS' ENTERED AT 13:39:10 ON 01 OCT 2002

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L26      9 S L10
L27      5 S L12
L28      5 S L14
L29      11 S L16
L30      7 S L18
          DEL HAR722E/A

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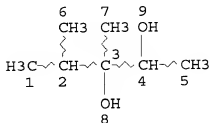
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SAV L16 HAR772E/A

FILE 'REGISTRY' ENTERED AT 13:45:14 ON 01 OCT 2002

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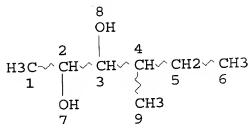
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STEREO ATTRIBUTES: NONE  
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3 ANSWERS

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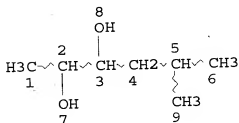
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11 ANSWERS

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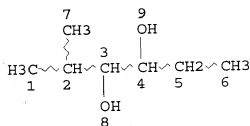
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1 ANSWERS

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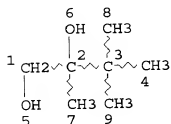
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STEREO ATTRIBUTES: NONE  
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1 ANSWERS

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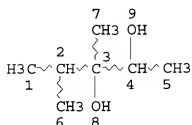
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STEREO ATTRIBUTES: NONE  
L16 3 SEA FILE=REGISTRY FAM FUL L5

100.0% PROCESSED 1006 ITERATIONS  
SEARCH TIME: 00.00.01

3 ANSWERS

=> d l18 que stat  
L6 STR



NODE ATTRIBUTES:  
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE  
L18 3 SEA FILE=REGISTRY FAM FUL L6

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3 ANSWERS

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FILE COVERS 1907 - 1 Oct 2002 VOL 137 ISS 14  
FILE LAST UPDATED: 30 Sep 2002 (20020930/ED)

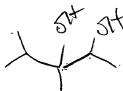
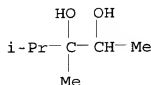
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=> d 125 1-7 cbib abs hitstr hitrn

L25 ANSWER 1 OF 7 ZCAPLUS COPYRIGHT 2002 ACS  
2002:271975 Document No. 136:296571 Concentrated, water dispersible, stable, fabric softening compositions. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert; Vogel, Alice Marie (The Procter & Gamble Company, USA). U.S. US 6369025 B1 20020409, 43 pp., Cont.-in-part of U.S. Ser. No. 638,024. (English). CODEN: USXXAM. APPLICATION: US 1998-983544 19980427. PRIORITY: US 1995-PV1057 19950711; US 1996-621019 19960322; US 1996-638024 19960426; WO 1996-US11580 19960711.  
AB An aq., concd., stable, translucent, or preferably, clear, rinse added liq. fabric softening compn. provided excellent H2O dispersibility in rinse H2O, and comprises a fabric softening active and <40% principal solvent having a ClogP .apprx.0.15-0.64, and an asym. structure. Also, the compn. may contain <10% solvent selected from EtOH, isopropanol, propylene glycol, 1,3-propanediol, propylene carbonate, and mixts. In order to achieve excellent H2O dispersibility, the molar ratio of a principal solvent of a fabric softening active should be .gtoreq.3, preferably .apprx.3.6-100.  
IT 187727-33-9  
(concd., water dispersible, stable, fabric softening compns.)

RN 187727-33-9 ZCAPLUS  
 CN 2,3-Pentanediol, 3,4-dimethyl- (9CI) (CA INDEX NAME)



3,3  
 3,4-di. Me - 2,3

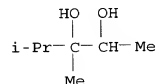
IT 187727-33-9  
 (concd., water dispersible, stable, fabric softening compns.)

L25 ANSWER 2 OF 7 ZCAPLUS COPYRIGHT 2002 ACS  
 2001:863494 Document No. 135:373284 Concentrated, stable clear fabric softening composition. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert; Vogel, Alice Marie (The Procter & Gamble Company, USA). U.S. US 6323172 B1 20011127, 126 pp., Cont.-in-part of U.S. Ser. No. 621,019, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1998-983542 19980925. PRIORITY: US 1996-621019 19960322; US 1996-620767 19960322; US 1996-620627 19960322; US 1996-620513 19960322; US 1996-621285 19960322; US 1996-621299 19960322; US 1996-621298 19960322; US 1996-620626 19960322; US 1996-620625 19960322; US 1996-620772 19960322; US 1996-621281 19960322; US 1996-620514 19960322; US 1996-620958 19960322; WO 1996-US11556 19960711.

AB The title fabric softener contains 2-80% actives that are either unsatd., or have intermediate length chains (C12-14) e.g. N,N-di(cocoyloxyethyl)-N,N-dimethylammonium chloride, and principal solvents (.ltorsim.40%), esp. mono-ol and diol principal solvents, having a ClogP .apprx.0.15-0.64, preferably .apprx.0.25-0.62, and more preferably .apprx.0.40-0.60, which are not sym., optionally low mol. wt. water-sol. solvents, and optionally water-sol. Ca and/or Mg salts, and the balance water. An example clear liq. softener contained N,N-di(cocoyloxyethyl)-N,N-dimethylammonium chloride 27.5, EtOH 5.1, 1,2-hexanediol 16%, HCl 0.005, Kathon 3 ppm, and the balance water.

IT 187727-33-9, 2,3-Pentanediol, 3,4-dimethyl-  
 (concn. aq. clear liq. fabric softening compn. contg.)

RN 187727-33-9 ZCAPLUS  
 CN 2,3-Pentanediol, 3,4-dimethyl- (9CI) (CA INDEX NAME)



IT 187727-33-9, 2,3-Pentanediol, 3,4-dimethyl-  
(concn. aq. clear liq. fabric softening compn. contg.)

L25 ANSWER 3 OF 7 ZCAPLUS COPYRIGHT 2002 ACS

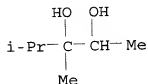
1998:268582 Document No. 128:323167 Concentrated aqueous clear liquid fabric softening composition. Wahl, Errol Hoffman; Trinh, Toan; Oler, Chad James (Procter & Gamble Co., USA; Wahl, Errol Hoffman; Trinh, Toan; Oler, Chad James). PCT Int. Appl. WO 9817756 A1 19980430, 153 pp. DESIGNATED STATES: W: BR, CA, CN, JP, MX, US. (English). CODEN: PIXXD2. APPLICATION: WO 1997-US18932 19971021. PRIORITY: US 1996-28904 19961021.

AB Principal solvents, esp. mono-ol and diol principal solvents, having a ClogP .apprx.0.15-0.64, preferably .apprx.0.25-0.62, and more preferably .apprx.0.40-0.60, have the ability to make clear aq. fabric softener compns. contg. relatively high concns. of fabric softener actives having highly unsatd. hydrocarbon moieties or branched chains in 2 long-chain hydrophobic groups with specific cis/trans ratios and having long chain hydrocarbon groups with an iodine value .apprx.70-140 for the unsatd. groups corresponding to fatty acids with the same no. of carbons and the same configuration. The title compn. contains .ltorsim.40% solvents and 2-80% fabric softener actives, prepd. in the presence of chelating agent and/or antioxidant with reduced coloration and malodor. Premixes of the fabric softening actives, the principal solvents, and, optionally, other solvents are a preferred means of adding actives to complete formulations.

IT 187727-33-9, 2,3-Pentanediol, 3,4-dimethyl-  
(concd. aq. clear liq. fabric softening compn. with reduced malodor and coloration)

RN 187727-33-9 ZCAPLUS

CN 2,3-Pentanediol, 3,4-dimethyl- (9CI) (CA INDEX NAME)



IT 187727-33-9, 2,3-Pentanediol, 3,4-dimethyl-  
(concd. aq. clear liq. fabric softening compn. with reduced malodor and coloration)

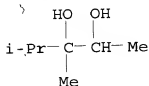
L25 ANSWER 4 OF 7 ZCAPLUS COPYRIGHT 2002 ACS

1997:224021 Document No. 126:213656 Concentrated, water dispersible, stable, fabric softening compositions. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo Jean-Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert; Vogel, Alice Marie; Rungta, Kamal Kumar; Sudarsana, Borra;

Okamoto, Mitsuyo; et al. (Procter and Gamble Company, USA; Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol, Hoffman; Rinker, Jennifer, Lea; Demeyere, Hugo, Jean-Marie; Declercq, Marc, Johan; Gosselink, Eugene, Paul). PCT Int. Appl. WO 9703170 A1 19970130, 111 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-US11580 19960711. PRIORITY: US 1995-1057 19950711; US 1996-621019 19960322; US 1996-638024 19960426.

AB The title aq., concd., stable, translucent, or preferably, clear, rinse added liq. fabric softening comps. which provide excellent water dispersibility in rinse water comprise a quaternary ammonium fabric softening active and a principal solvent of mainly diols or derivs. and mixts. thereof. To achieve the main object of excellent water dispersibility, the molar ratio of a principal solvent to a fabric softening active should be not less than 3, preferably from about 3.6-100, e.g., 1,2-hexanediol and dimethyldioleammonium chloride in 25.8:1 molar ratio, showing a homogeneous soln. in 50% diln. in cold water.

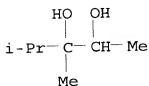
IT 187727-33-9  
(concd., water dispersible, stable, fabric softening comps.)  
RN 187727-33-9 ZCAPLUS  
CN 2,3-Pentanediol, 3,4-dimethyl- (9CI) (CA INDEX NAME)



IT 187727-33-9  
(concd., water dispersible, stable, fabric softening comps.)

L25 ANSWER 5 OF 7 ZCAPLUS COPYRIGHT 2002 ACS  
1997:215734 Document No. 126:200646 Solvents for concentrated, stable fabric softening composition. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Vogel, Alice Marie; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert (Procter and Gamble Company, USA; Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Vogel, Alice Marie; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; et al.). PCT Int. Appl. WO 9703169 A1 19970130, 277 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG; RW: AT, BE, BF, BJ, CF, CG,

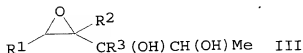
- CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-US11556 19960711. PRIORITY: US 1995-1057 19950711; US 1996-621019 19960322.
- AB Principal solvents, esp. monoools and diols, having a ClogP (calcd. logP, where P is the octanol-water partition coeff. of the substance) of 0.15-0.64, have the ability to make clear aq. fabric softener compns. contg. relatively high concns. of fabric softener actives having ester linkages in their long, hydrophobic chains. The fabric softener actives are either unsatd., or have intermediate length chains (.apprx.C12-14) and the principal solvents are used at levels of less than about 40 %. Other solvents may be present. Some of the principal solvents are novel compds. and/or novel mixts. Premixes of the fabric softening actives, the principal solvents, and, optionally, other solvents are useful in the prepn. of complete formulation by obviating/limiting the need for heating.
- IT 187727-33-9  
(solvents for concd., stable fabric softening compn.)
- RN 187727-33-9 ZCAPLUS
- CN 2,3-Pentanediol, 3,4-dimethyl- (9CI) (CA INDEX NAME)



- IT 187727-33-9  
(solvents for concd., stable fabric softening compn.)

L25 ANSWER 6 OF 7 ZCAPLUS COPYRIGHT 2002 ACS  
1993:560002 Document No. 119:160002 Direct epoxy hydroxylation of hydroperoxy homoallylic alcohols: multidentate oxygen donor and oxygen acceptor substrates in titanium(IV)-catalyzed epoxidations. Adam, Waldemar; Nestler, Bernd (Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, D-8700, Germany). Journal of the American Chemical Society, 115(16), 7226-31 (English) 1993. CODEN: JACSAT. ISSN: 0002-7863.

GI



- AB The hydroperoxy homoallylic alcs. (R\*,S\*)-CH<sub>2</sub>:CMeCH(OOH)CH(OH)Me and (S\*,S\*)-R<sub>1</sub>CH:CR<sub>2</sub>CR<sub>3</sub>(OOH)CH(OH)Me (I; R<sub>1</sub> = H, Bu; R<sub>2</sub>, R<sub>3</sub> = H, Me), readily available through the photooxygenation of chiral allylic

alcs. R1CH2CR2:CR3CH(OH)Me (II), were converted to epoxy diols (III) under the catalytic action of Ti(OCHMe2)4. In these epoxy hydroxylations, the hydroperoxides play a double role as oxygen atom donor and, in the form of the in situ generated corresponding unsatd. diols (IV), as substrate for oxygen transfer. Compared to Ti(IV)-catalyzed epoxidns. of unsatd. diols by tert-BuOOH, the advantage of this approach is that a large rate enhancement is obtained. Moreover, with the exception of I (R1 = R2 = H, R3 = Me), all reactions proceeded with unusually high diastereoselectivity. These results are rationalized in terms of the ability of the hydroxy-functionalized hydroperoxides (oxygen atom donors) as well as IV (oxygen atom acceptors) to chelate to the titanium metal in the catalytically operating template. For some IV bidentate binding is feasible, while for other IV this is difficult due to unfavorable steric interactions. Important for synthetic applications is the fact that II can be directly converted to III in a one-pot, two-step procedure simply by adding catalytic amts. of Ti(OCHMe2)4 to a photooxygenated soln. of II.

IT 150129-17-2

(reaction of, with titanium tetra-tert-butoxide)

RN 150129-17-2 ZCAPLUS

IT 150129-17-2 (reaction of, with titanium tetra-tert-butoxide)

L25 ANSWER 7 OF 7 ZCAPLUS COPYRIGHT 2002 ACS

1973:97026 Document No. 78:97026 Stereoselectivity in the reduction of aliphatic .alpha.-ketols with aluminum hydride reagents.

Katzenellenbogen, John A.; Bowlus, Stephen B. (Dep. Chem., Univ. Illinois, Urbana) Ill., USA). J. Org. Chem., 38(4), 627-32 (English) 1973. CODEN: JOCEAH.

AB Redn. of 8 .alpha.-ketols with different patterns of substitution and size of substituents was investigated using 7 Al hydride reagents. The ratio of diastereomeric diols produced was detd. by 220 MHz NMR anal. In each case the predominant diol was the one predicted by Cram's cyclic model. The degree of stereoselectivity correlates well with .alpha.-ketol structure with only 1 reagent (triisobutylaluminum). With the other (agglomerated) reagents, selectivity is related only in an irregular manner to .alpha.-ketol structure.

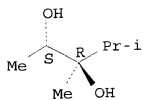
IT 37164-04-8P 37164-05-9P

(prepn. and configuration of, NMR in relation to)

RN 37164-04-8 ZCAPLUS

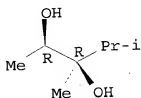
CN 2,3-Pentanediol, 3,4-dimethyl-, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 37164-05-9 ZCAPLUS  
 CN 2,3-Pentandiol, 3,4-dimethyl-, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 37164-04-8P 37164-05-9P  
 (prepn. and configuration of, NMR in relation to)



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L26 ANSWER 1 OF 9 ZCAPLUS COPYRIGHT 2002 ACS

2002:271975 Document No. 136:296571 Concentrated, water dispersible, stable, fabric softening compositions. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert; Vogel, Alice Marie (The Procter & Gamble Company, USA). U.S. US 6369025 B1 20020409, 43 pp., Cont.-in-part of U.S. Ser. No. 638,024. (English). CODEN: USXXAM. APPLICATION: US 1998-983544 19980427. PRIORITY: US 1995-PV1057 19950711; US 1996-621019 19960322; US 1996-638024 19960426; WO 1996-US11580 19960711.

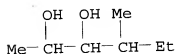
AB An aq., concd., stable, translucent, or preferably, clear, rinse added liq. fabric softening compn. provided excellent H2O dispersibility in rinse H2O, and comprises a fabric softening active and <40% principal solvent having a ClogP .apprx.0.15-0.64, and an asym. structure. Also, the compn. may contain <10% solvent selected from EtOH, isopropanol, propylene glycol, 1,3-propanediol, propylene carbonate, and mixts. In order to achieve excellent H2O dispersibility, the molar ratio of a principal solvent of a fabric softening active should be .gtoreq.3, preferably .apprx.3.6-100.

IT 187727-35-1

(conc'd., water dispersible, stable, fabric softening compns.)

RN 187727-35-1 ZCAPLUS

CN 2,3-Hexanediol, 4-methyl- (9CI) (CA INDEX NAME)



IT 187727-35-1

(conc'd., water dispersible, stable, fabric softening compns.)

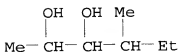
L26 ANSWER 2 OF 9 ZCAPLUS COPYRIGHT 2002 ACS

2001:863494 Document No. 135:373284 Concentrated, stable clear fabric softening composition. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert; Vogel, Alice Marie (The Procter & Gamble Company, USA). U.S. US 6323172 B1 20011127, 126 pp., Cont.-in-part of U.S. Ser. No. 621,019, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1998-983542 19980925. PRIORITY: US 1996-621019 19960322; US 1996-620767 19960322; US 1996-620627 19960322; US 1996-620513 19960322; US 1996-621285 19960322; US 1996-621299 19960322; US 1996-621298 19960322; US 1996-620626 19960322; US 1996-620625 19960322; US 1996-620772 19960322; US 1996-621281 19960322; US 1996-620514 19960322; US 1996-620958 19960322; WO 1996-US11556 19960711.

AB The title fabric softener contains 2-80% actives that are either

unsatd., or have intermediate length chains (C12-14 ) e.g. N,N-di(cocooxyethyl)-N,N-dimethylammonium chloride, and principal solvents (.ltorsim.40%), esp. mono-ol and diol principal solvents, having a ClogP .apprx.0.15-0.64, preferably .apprx.0.25-0.62, and more preferably .apprx.0.40-0.60, which are not sym., optionally low mol. wt. water-sol. solvents, and optionally water-sol. Ca and/or Mg salts, and the balance water. An example clear liq. softener contained N,N-di(cocooxyethyl)-N,N-dimethylammonium chloride 27.5, EtOH 5.1, 1,2-hexanediol 16%, HCl 0.005, Kathon 3 ppm, and the balance water.

IT 187727-35-1, 2,3-Hexanediol, 4-methyl-  
(concn. aq. clear liq. fabric softening compn. contg.)  
RN 187727-35-1 ZCAPLUS  
CN 2,3-Hexanediol, 4-methyl- (9CI) (CA INDEX NAME)



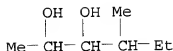
IT 187727-35-1, 2,3-Hexanediol, 4-methyl-  
(concn. aq. clear liq. fabric softening compn. contg.)

L26 ANSWER 3 OF 9 ZCAPLUS COPYRIGHT 2002 ACS

1998:268582 Document No. 128:323167 Concentrated aqueous clear liquid fabric softening composition. Wahl, Errol Hoffman; Trinh, Toan; Oler, Chad James (Procter & Gamble Co., USA; Wahl, Errol Hoffman; Trinh, Toan; Oler, Chad James). PCT Int. Appl. WO 9817756 A1 19980430, 153 pp. DESIGNATED STATES: W: BR, CA, CN, JP, MX, US. (English). CODEN: PIXXD2. APPLICATION: WO 1997-US18932 19971021. PRIORITY: US 1996-28904 19961021.

AB Principal solvents, esp. mono-ol and diol principal solvents, having a ClogP .apprx.0.15-0.64, preferably .apprx.0.25-0.62, and more preferably .apprx.0.40-0.60, have the ability to make clear aq. fabric softener compns. contg. relatively high concns. of fabric softener actives having highly unsatd. hydrocarbon moieties or branched chains in 2 long-chain hydrophobic groups with specific cis/trans ratios and having long chain hydrocarbon groups with an iodine value .apprx.70-140 for the unsatd. groups corresponding to fatty acids with the same no. of carbons and the same configuration. The title compn. contains .ltorsim.40% solvents and 2-80% fabric softener actives, prepd. in the presence of chelating agent and/or antioxidant with reduced coloration and malodor. Premixes of the fabric softening actives, the principal solvents, and, optionally, other solvents are a preferred means of adding actives to complete formulations.

IT 187727-35-1, 2,3-Hexanediol, 4-methyl-  
(concd. aq. clear liq. fabric softening compn. with reduced  
malodor and coloration)  
RN 187727-35-1 ZCAPLUS  
CN 2,3-Hexanediol, 4-methyl- (9CI) (CA INDEX NAME)



IT 187727-35-1, 2,3-Hexanediol, 4-methyl-  
(concd. aq. clear liq. fabric softening compn. with reduced  
malodor and coloration)

L26 ANSWER 4 OF 9 ZCAPLUS COPYRIGHT 2002 ACS

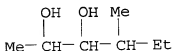
1997:224021 Document No. 126:213656 Concentrated, water dispersible,  
stable, fabric softening compositions. Trinh, Toan; Tordil, Helen  
Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo  
Jean-Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton,  
James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark  
Robert; Vogel, Alice Marie; Rungta, Kamal Kumar; Sudarsana, Borra;  
Okamoto, Mitsuyo; et al. (Procter and Gamble Company, USA; Trinh,  
Toan; Tordil, Helen Bernardo; Wahl, Errol, Hoffman; Rinker,  
Jennifer, Lea; Demeyere, Hugo, Jean-Marie; Declercq, Marc, Johan;  
Gosselink, Eugene, Paul). PCT Int. Appl. WO 9703170 A1 19970130,  
111 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY,  
CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG,  
KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ,  
PL, PT, RO, RU, SD, SE, SG; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM,  
DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE.  
(English). CODEN: PIXXD2. APPLICATION: WO 1996-US11580 19960711.  
PRIORITY: US 1995-1057 19950711; US 1996-621019 19960322; US  
1996-638024 19960426.

AB The title aq., concd., stable, translucent, or preferably, clear,  
rinse added liq. fabric softening compns. which provide excellent  
water dispersibility in rinse water comprise a quaternary ammonium  
fabric softening active and a principal solvent of mainly diols or  
derivs. and mixts. thereof. To achieve the main object of excellent  
water dispersibility, the molar ratio of a principal solvent to a  
fabric softening active should be not less than 3, preferably from  
about 3.6-100, e.g., 1,2-hexanediol and dimethyldioleyleammonium  
chloride in 25.8:1 molar ratio, showing a homogeneous soln. in 50%  
dilm. in cold water.

IT 187727-35-1  
(concd., water dispersible, stable, fabric softening compns.)

RN 187727-35-1 ZCAPLUS

CN 2,3-Hexanediol, 4-methyl- (9CI) (CA INDEX NAME)



IT 187727-35-1

(concd., water dispersible, stable, fabric softening compns.)

L26 ANSWER 5 OF 9 ZCAPLUS COPYRIGHT 2002 ACS

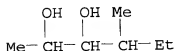
1997:215734 Document No. 126:200646 Solvents for concentrated, stable fabric softening composition. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Vogel, Alice Marie; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert (Procter and Gamble Company, USA; Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Vogel, Alice Marie; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; et al.). PCT Int. Appl. WO 9703169 A1 19970130, 277 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-US11556

AB 19960711. PRIORITY: US 1995-1057 19950711; US 1996-621019 19960322. Principal solvents, esp. monools and diols, having a ClogP (calcd. logP, where P is the octanol-water partition coeff. of the substance) of 0.15-0.64, have the ability to make clear aq. fabric softener compns. contg. relatively high concns. of fabric softener actives having ester linkages in their long, hydrophobic chains. The fabric softener actives are either unsatd., or have intermediate length chains (.apprx.C12-14) and the principal solvents are used at levels of less than about 40 %. Other solvents may be present. Some of the principal solvents are novel compds. and/or novel mixts. Premixes of the fabric softening actives, the principal solvents, and, optionally, other solvents are useful in the prepn. of complete formulation by obviating/limiting the need for heating.

IT 187727-35-1 (solvents for concd., stable fabric softening compn.)

RN 187727-35-1 ZCAPLUS

CN 2,3-Hexanediol, 4-methyl- (9CI) (CA INDEX NAME)



IT 187727-35-1

(solvents for concd., stable fabric softening compn.)

L26 ANSWER 6 OF 9 ZCAPLUS COPYRIGHT 2002 ACS

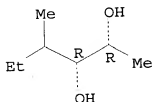
1996:705636 Document No. 126:46787 Comparative Diastereoselectivity Analysis of Crotylindium and 3-Bromoallylindium Additions to .alpha.-Oxy Aldehydes in Aqueous and Nonaqueous Solvent Systems. Paquette, Leo A.; Mitzel, Thomas M. (Evans Chemical Laboratories, Ohio State University, Columbus, OH, 43210, USA). Journal of Organic Chemistry, 61(25), 8799-8804 (English) 1996. CODEN: JOCEAH.

ISSN: 0022-3263. OTHER SOURCES: CASREACT 126:46787. Publisher: American Chemical Society.

AB The couplings of crotyl bromide (1) and 1,3-dibromopropene (2) to a triad of conformationally unrestricted .alpha.-oxy aldehydes in water, aq. THF (1:1), and anhyd. THF are described. In no example involving 1 was the formation of anti,syn product detected. The proportion of syn isomers reached a max. (syn/anti = 5.6:1) when the neighboring hydroxyl group was unprotected and water was the reaction medium. Although internal chelation also operates to some degree with 2, considerable erosion of this mechanistic pathway (max. now only 2:1) in favor of Felkin and "anti-Felkin" transition states is reflected in the product distributions. This trend can be synthetically advantageous, and a utilitarian example is demonstrated. The indium reagents studied here are notably efficient nucleophilic reaction partners in water.

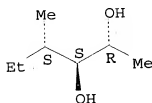
IT 184897-19-6P 184897-21-0P  
(stereochem. of addn. of crotylindium and 3-bromoallylindium to .alpha.-oxy aldehydes in aq. and nonaq. solvent systems)  
RN 184897-19-6 ZCAPLUS  
CN 2,3-Hexanediol, 4-methyl-, (2R,3R)-rel-[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 184897-21-0 ZCAPLUS  
CN 2,3-Hexanediol, 4-methyl-, (2R\*,3S\*,4S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

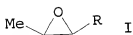


IT 184897-19-6P 184897-21-0P  
(stereochem. of addn. of crotylindium and 3-bromoallylindium to .alpha.-oxy aldehydes in aq. and nonaq. solvent systems)

L26 ANSWER 7 OF 9 ZCAPLUS COPYRIGHT 2002 ACS  
1993:168901 Document No. 118:168901 Enantio- and regioselectivity in the epoxide-hydrolase-catalyzed ring opening of aliphatic oxiranes:

Part II: Dialkyl- and trialkyl-substituted oxiranes. Wistuba, D.; Traeger, O.; Schurig, V. (Inst. Org. Chem., Univ. Tuebingen, Tuebingen, Germany). Chirality, 4(3), 185-92 (English) 1992. CODEN: CHRLEP. ISSN: 0899-0042.

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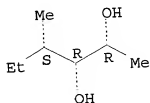
AB The extent of substrate enantioselectivity and regioselectivity of a series of aliph. 2,3-dialkyl- and trialkylsubstituted oxiranes in their in vitro epoxide-hydrolase-catalyzed hydrolysis depends on the size of the alkyl residues and on the substitution pattern of the oxirane ring. The enzyme-catalyzed hydrolysis of cis-oxiranes I (R = Me, Et, sec-Bu), contg. at least one Me substituent, shows complete or nearly complete substrate enantioselectivity and regioselectivity with nucleophilic attack by water occurring with inversion of configuration at the methylsubstituted ring carbon atom of (S)-configuration. In the hydrolysis of the isomeric trans-oxiranes, both enantiomers are metabolized with a higher rate for the (2S;3S)-enantiomer. The conversion of trimethyloxirane occurs with high substrate enantioselectivity in favor of the (S)-enantiomer and with complete regioselectivity at the monomethylsubstituted ring carbon atom. The differentiation of the enantiotopic ring carbon atoms (product enantioselectivity) in the smallest aliph. meso-oxirane, cis-2,3-dimethyloxirane, leads to (2R;3R)-butane-2,3-diol with ee = 86%. cis-2-Ethyl-3-propyloxirane, possessing alkyl residues larger than Me, represents an extremely poor substrate in the epoxide-hydrolase-catalyzed hydrolysis process.

IT 146452-48-4P 146452-49-5P 146452-50-8P  
146452-51-9P

(prepn. of)

RN 146452-48-4 ZCAPLUS  
CN 2,3-Hexanediol, 4-methyl-, [2R-(2R\*,3R\*,4S\*)]- (9CI) (CA INDEX NAME)

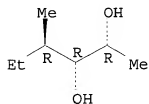
Absolute stereochemistry.



RN 146452-49-5 ZCAPLUS  
CN 2,3-Hexanediol, 4-methyl-, [2R-(2R\*,3R\*,4R\*)]- (9CI) (CA INDEX NAME)

(NAME)

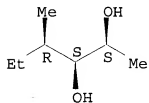
Absolute stereochemistry.



RN 146452-50-8 ZCAPLUS

CN 2,3-Hexanediol, 4-methyl-, [2S-(2R\*,3R\*,4S\*)]- (9CI) (CA INDEX NAME)

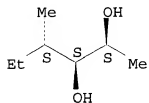
Absolute stereochemistry.



RN 146452-51-9 ZCAPLUS

CN 2,3-Hexanediol, 4-methyl-, [2S-(2R\*,3R\*,4R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

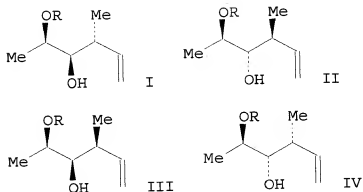


IT 146452-48-4P 146452-49-5P 146452-50-8P  
 146452-51-9P  
 (prepn. of)

L26 ANSWER 8 OF 9 ZCAPLUS COPYRIGHT 2002 ACS

1990:7655 Document No. 112:7655 Stereochemical aspects of the  
 additions of anti-selective, crotyl organometallic reagents to  
 .alpha.-alkoxy aldehydes. Martin, Stephen F.; Li, Wei (Dep. Chem.,  
 Univ. Texas, Austin, TX, 78712, USA). J. Org. Chem., 54(26),  
 6129-33 (English) 1989. CODEN: JOCEAH. ISSN: 0022-3263. OTHER  
 SOURCES: CASREACT 112:7655.

GI



AB The nucleophilic addns. of a variety of anti-selective crotyl organometallic reagents  $\text{MeCH:CHCH}_2\text{M}$  [ $\text{M} = \text{Cp}_2\text{TiCl}$  ( $\text{Cp} = \text{eta}^5\text{-cyclopentadienyl}$ ),  $\text{Ti}(\text{OPh})_3$ ,  $\text{Cp}_2\text{ZrCl}$ ,  $\text{CrCl}$ , and  $\text{CrCl}_2$ ] to .alpha.-alkoxy aldehydes,  $\text{MeCH(OR)CHO}$  ( $\text{R} = \text{PhCH}_2$ ,  $\text{PhCH}_2\text{OCH}_2$ ,  $\text{Me}_2\text{SiCMe}_3$ ,  $\text{MeOCH}_2\text{CH}_2\text{OCH}_2$ ,  $\text{Ph}_3\text{C}$ ) were examd. to ascertain whether high levels of diastereoselectivity could be achieved via a chelation-controlled transition state. Although the anti-adducts I and II dominated (2 to >100:1) over the corresponding syn-adducts III and IV, the ratios of chelation controlled products I and III to the non-chelation controlled products II and IV varied from 0.8 to 1.8:1.

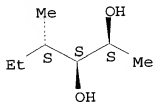
IT 123807-31-8P 123807-32-9P 123807-33-0P  
123807-34-1P

(prepn. of)

RN 123807-31-8 ZCAPLUS

CN 2,3-Hexanediol, 4-methyl-, (2R\*,3R\*,4R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



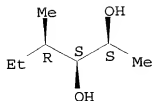
RN 123807-32-9 ZCAPLUS

RN 123807-33-0 ZCAPLUS

CN 2,3-Hexanediol, 4-methyl-, (2R\*,3R\*,4S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

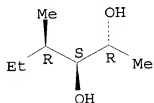




RN 123807-34-1 ZCAPLUS

CN 2,3-Hexanediol, 4-methyl-, (2R\*,3S\*,4R\*)- (9CI) (CA INDEX NAME)

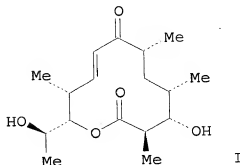
Relative stereochemistry.



IT 123807-31-8P 123807-32-9P 123807-33-0P  
 123807-34-1P  
 (prepn. of)

L26 ANSWER 9 OF 9 ZCAPLUS COPYRIGHT 2002 ACS  
 1987:18204 Document No. 106:18204 Total synthesis of neomethynolide.  
 Inanaga, Junji; Kawanami, Yasuhiro; Yamaguchi, Masaru (Fac. Sci.,  
 Kyushu Univ., Fukuoka, 812, Japan). Bull. Chem. Soc. Jpn., 59(5),  
 1521-8 (English) 1986. CODEN: BCSJAB. ISSN: 0009-2673. OTHER  
 SOURCES: CASREACT 106:18204.

GI



AB (+)-Neomethynolide (I), the aglycon of, neomethymycin, was totally synthesized. The construction of the skeleton was carried out by condensing a stereoselectivity synthesized fragment,

4-(tert-butyldimethylsiloxy)-5-[(2-methoxyethoxy)methoxy]-3-methyl-1-hexyne, with Prelog-Djerassi lactonic ester, and the mixed anhydride method was used for the lactonization of an intermediate hydroxy acid. The full stereochem. of I was established by this synthesis.

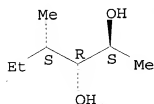
IT 105827-03-0P

(prepn. of)

RN 105827-03-0 ZCAPLUS

CN 2,3-Hexanediol, 4-methyl-, [2S-(2R\*,3S\*,4R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 105827-03-0P  
(prepn. of)

=> d 127 1-5 cbib abs hitstr hitrn

L27 ANSWER 1 OF 5 ZCAPLUS COPYRIGHT 2002 ACS

2002:271975 Document No. 136:296571 Concentrated, water dispersible, stable, fabric softening compositions. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert; Vogel, Alice Marie (The Procter & Gamble Company, USA). U.S. US 6369025 B1 20020409, 43 pp., Cont.-in-part of U.S. Ser. No. 638,024. (English). CODEN: USXXAM. APPLICATION: US 1998-983544 19980427. PRIORITY: US 1995-PV1057 19950711; US 1996-621019 19960322; US 1996-638024 19960426; WO 1996-US11580 19960711.

AB An aq., concd., stable, translucent, or preferably, clear, rinse added liq. fabric softening compn. provided excellent H2O dispersibility in rinse H2O, and comprises a fabric softening active and <40% principal solvent having a ClogP .apprx.0.15-0.64, and an asym. structure. Also, the compn. may contain <10% solvent selected from EtOH, isopropanol, propylene glycol, 1,3-propanediol, propylene carbonate, and mixts. In order to achieve excellent H2O dispersibility, the molar ratio of a principal solvent of a fabric softening active should be .gtoreq.3, preferably .apprx.3.6-100.

IT 187727-38-4

(concd., water dispersible, stable, fabric softening compns.)

RN 187727-38-4 ZCAPLUS

CN 2,3-Hexanediol, 5-methyl- (9CI) (CA INDEX NAME)

OH OH

Me-CH-CH-Bu-i

IT 187727-38-4

(concd., water dispersible, stable, fabric softening compns.)

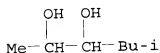
L27 ANSWER 2 OF 5 ZCAPLUS COPYRIGHT 2002 ACS

2001:863494 Document No. 135:373284 Concentrated, stable clear fabric softening composition. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert; Vogel, Alice Marie (The Procter & Gamble Company, USA). U.S. US 6323172 B1 20011127, 126 pp., Cont.-in-part of U.S. Ser. No. 621,019, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1998-983542 19980925. PRIORITY: US 1996-621019 19960322; US 1996-620767 19960322; US 1996-620627 19960322; US 1996-620513 19960322; US 1996-621285 19960322; US 1996-621299 19960322; US 1996-621298 19960322; US 1996-620626 19960322; US 1996-620625 19960322; US 1996-620772 19960322; US 1996-621281 19960322; US 1996-620514 19960322; US 1996-620958 19960322; WO 1996-US11556 19960711.

AB The title fabric softener contains 2-80% actives that are either

unsatd., or have intermediate length chains (C12-14 ) e.g. N,N-di(cocoxyloxyethyl)-N,N-dimethylammonium chloride, and principal solvents (.ltorsim.40%), esp. mono-ol and diol principal solvents, having a ClogP .apprx.0.15-0.64, preferably .apprx.0.25-0.62, and more preferably .apprx.0.40-0.60, which are not sym., optionally low mol. wt. water-sol. solvents, and optionally water-sol. Ca and/or Mg salts, and the balance water. An example clear liq. softener contained N,N-di(cocoxyloxyethyl)-N,N-dimethylammonium chloride 27.5, EtOH 5.1, 1,2-hexanediol 16%, HCl 0.005, Kathon 3 ppm, and the balance water.

IT 187727-38-4, 2,3-Hexanediol, 5-methyl-  
(concn. aq. clear liq. fabric softening compn. contg.)  
RN 187727-38-4 ZCAPLUS  
CN 2,3-Hexanediol, 5-methyl- (9CI) (CA INDEX NAME)

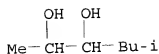


IT 187727-38-4, 2,3-Hexanediol, 5-methyl-  
(concn. aq. clear liq. fabric softening compn. contg.)

L27 ANSWER 3 OF 5 ZCAPLUS COPYRIGHT 2002 ACS  
1998:268582 Document No. 128:323167 Concentrated aqueous clear liquid fabric softening composition. Wahl, Errol Hoffman; Trinh, Toan; Oler, Chad James (Procter & Gamble Co., USA; Wahl, Errol Hoffman; Trinh, Toan; Oler, Chad James). PCT Int. Appl. WO 9817756 A1 19980430, 153 pp. DESIGNATED STATES: W: BR, CA, CN, JP, MX, US. (English). CODEN: PIXXD2. APPLICATION: WO 1997-US18932 19971021. PRIORITY: US 1996-28904 19961021.

AB Principal solvents, esp. mono-ol and diol principal solvents, having a ClogP .apprx.0.15-0.64, preferably .apprx.0.25-0.62, and more preferably .apprx.0.40-0.60, have the ability to make clear aq. fabric softener compns. contg. relatively high concns. of fabric softener actives having highly unsatd. hydrocarbon moieties or branched chains in 2 long-chain hydrophobic groups with specific cis/trans ratios and having long chain hydrocarbon groups with an iodine value .apprx.70-140 for the unsatd. groups corresponding to fatty acids with the same no. of carbons and the same configuration. The title compn. contains .ltorsim.40% solvents and 2-80% fabric softener actives, prepd. in the presence of chelating agent and/or antioxidant with reduced coloration and malodor. Premixes of the fabric softening actives, the principal solvents, and, optionally, other solvents are a preferred means of adding actives to complete formulations.

IT 187727-38-4, 2,3-Hexanediol, 5-methyl-  
(concd. aq. clear liq. fabric softening compn. with reduced malodor and coloration)  
RN 187727-38-4 ZCAPLUS  
CN 2,3-Hexanediol, 5-methyl- (9CI) (CA INDEX NAME)

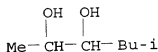


IT 187727-38-4, 2,3-Hexanediol, 5-methyl-  
(concd. aq. clear liq. fabric softening compn. with reduced  
malodor and coloration)

L27 ANSWER 4 OF 5 ZCAPLUS COPYRIGHT 2002 ACS  
1997:224021 Document No. 126:213656 Concentrated, water dispersible,  
stable, fabric softening compositions. Trinh, Toan; Tordil, Helen  
Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo  
Jean-Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton,  
James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark  
Robert; Vogel, Alice Marie; Rungta, Kamal Kumar; Sudarsana, Borra;  
Okamoto, Mitsuyo; et al. (Procter and Gamble Company, USA; Trinh,  
Toan; Tordil, Helen Bernardo; Wahl, Errol, Hoffman; Rinker,  
Jennifer, Lea; Demeyere, Hugo, Jean-Marie; Declercq, Marc, Johan;  
Gosselink, Eugene, Paul). PCT Int. Appl. WO 9703170 A1 19970130,  
111 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY,  
CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG,  
KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ,  
PL, PT, RO, RU, SD, SE, SG; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM,  
DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE.  
(English). CODEN: PIXXD2. APPLICATION: WO 1996-US11580 19960711.  
PRIORITY: US 1995-1057 19950711; US 1996-621019 19960322; US  
1996-638024 19960426.

AB The title aq., concd., stable, translucent, or preferably, clear,  
rinse added liq. fabric softening compns. which provide excellent  
water dispersibility in rinse water comprise a quaternary ammonium  
fabric softening active and a principal solvent of mainly diols or  
derivs. and mixts. thereof. To achieve the main object of excellent  
water dispersibility, the molar ratio of a principal solvent to a  
fabric softening active should be not less than 3, preferably from  
about 3.6-100, e.g., 1,2-hexanediol and dimethyldioleyleammonium  
chloride in 25.8:1 molar ratio, showing a homogeneous soln. in 50%  
diln. in cold water.

IT 187727-38-4  
(concd., water dispersible, stable, fabric softening compns.)  
RN 187727-38-4 ZCAPLUS  
CN 2,3-Hexanediol, 5-methyl- (9CI) (CA INDEX NAME)



IT 187727-38-4

(concd., water dispersible, stable, fabric softening compns.)

L27 ANSWER 5 OF 5 ZCAPLUS COPYRIGHT 2002 ACS

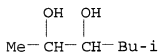
1997:215734 Document No. 126:200646 Solvents for concentrated, stable fabric softening composition. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Vogel, Alice Marie; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert (Procter and Gamble Company, USA; Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Vogel, Alice Marie; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; et al.). PCT Int. Appl. WO 9703169 A1 19970130, 277 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LJ, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-US11556

AB 19960711. PRIORITY: US 1995-1057 19950711; US 1996-621019 19960322. Principal solvents, esp. monools and diols, having a ClogP (calcd. logP, where P is the octanol-water partition coeff. of the substance) of 0.15-0.64, have the ability to make clear aq. fabric softener compns. contg. relatively high concns. of fabric softener actives having ester linkages in their long, hydrophobic chains. The fabric softener actives are either unsatd., or have intermediate length chains (.apprx.C12-14) and the principal solvents are used at levels of less than about 40 %. Other solvents may be present. Some of the principal solvents are novel compds. and/or novel mixts. Premixes of the fabric softening actives, the principal solvents, and, optionally, other solvents are useful in the prepn. of complete formulation by obviating/limiting the need for heating.

IT 187727-38-4 (solvents for concd., stable fabric softening compn.)

RN 187727-38-4 ZCAPLUS

CN 2,3-Hexanediol, 5-methyl- (9CI) (CA INDEX NAME)



IT 187727-38-4 (solvents for concd., stable fabric softening compn.)

=&gt; d 128 1-5 cbib abs hitstr hitrn

L28 ANSWER 1 OF 5 ZCAPLUS COPYRIGHT 2002 ACS

2002:271975 Document No. 136:296571 Concentrated, water dispersible, stable, fabric softening compositions. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert; Vogel, Alice Marie (The Procter & Gamble Company, USA). U.S. US 6369025 B1 20020409, 43 pp., Cont.-in-part of U.S. Ser. No. 638,024. (English). CODEN: USXXAM. APPLICATION: US 1998-983544 19980427. PRIORITY: US 1995-PV1057 19950711; US 1996-621019 19960322; US 1996-638024 19960426; WO 1996-US11580 19960711.

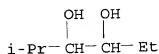
AB An aq., concd., stable, translucent, or preferably, clear, rinse added liq. fabric softening compn. provided excellent H2O dispersibility in rinse H2O, and comprises a fabric softening active and <40% principal solvent having a ClogP .apprx.0.15-0.64, and an asym. structure. Also, the compn. may contain <10% solvent selected from EtOH, isopropanol, propylene glycol, 1,3-propanediol, propylene carbonate, and mixts. In order to achieve excellent H2O dispersibility, the molar ratio of a principal solvent of a fabric softening active should be .gtoreq.3, preferably .apprx.3.6-100.

IT 187727-40-8

(concd., water dispersible, stable, fabric softening compns.)

RN 187727-40-8 ZCAPLUS

CN 3,4-Hexanediol, 2-methyl- (9CI) (CA INDEX NAME)



IT 187727-40-8

(concd., water dispersible, stable, fabric softening compns.)

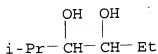
L28 ANSWER 2 OF 5 ZCAPLUS COPYRIGHT 2002 ACS

2001:863494 Document No. 135:373284 Concentrated, stable clear fabric softening composition. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert; Vogel, Alice Marie (The Procter & Gamble Company, USA). U.S. US 6323172 B1 20011127, 126 pp., Cont.-in-part of U.S. Ser. No. 621,019, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1998-983542 19980925. PRIORITY: US 1996-621019 19960322; US 1996-620767 19960322; US 1996-620627 19960322; US 1996-620513 19960322; US 1996-621285 19960322; US 1996-621299 19960322; US 1996-621298 19960322; US 1996-620626 19960322; US 1996-620625 19960322; US 1996-620772 19960322; US 1996-621281 19960322; US 1996-620514 19960322; US 1996-620958 19960322; WO 1996-US11556 19960711.

AB The title fabric softener contains 2-80% actives that are either

unsatd., or have intermediate length chains (C12-14) e.g. N,N-di(cocooxyloxyethyl)-N,N-dimethylammonium chloride, and principal solvents (.ltorsim.40%), esp. mono-ol and diol principal solvents, having a ClogP .apprx.0.15-0.64, preferably .apprx.0.25-0.62, and more preferably .apprx.0.40-0.60, which are not sym., optionally low mol. wt. water-sol. solvents, and optionally water-sol. Ca and/or Mg salts, and the balance water. An example clear liq. softener contained N,N-di(cocooxyloxyethyl)-N,N-dimethylammonium chloride 27.5, EtOH 5.1, 1,2-hexanediol 16%, HCl 0.005, Kathon 3 ppm, and the balance water.

IT 187727-40-8, 3,4-Hexanediol, 2-methyl-  
(concn. aq. clear liq. fabric softening compn. contg.)  
RN 187727-40-8 ZCAPLUS  
CN 3,4-Hexanediol, 2-methyl- (9CI) (CA INDEX NAME)



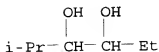
IT 187727-40-8, 3,4-Hexanediol, 2-methyl-  
(concn. aq. clear liq. fabric softening compn. contg.)

L28 ANSWER 3 OF 5 ZCAPLUS COPYRIGHT 2002 ACS  
1998:268582 Document No. 128:323167 Concentrated aqueous clear liquid fabric softening composition. Wahl, Errol Hoffman; Trinh, Toan; Oler, Chad James (Procter & Gamble Co., USA; Wahl, Errol Hoffman; Trinh, Toan; Oler, Chad James). PCT Int. Appl. WO 9817756 A1 19980430, 153 pp. DESIGNATED STATES: W: BR, CA, CN, JP, MX, US. (English). CODEN: PIXXD2. APPLICATION: WO 1997-US18932 19971021. PRIORITY: US 1996-28904 19961021.

AB Principal solvents, esp. mono-ol and diol principal solvents, having a ClogP .apprx.0.15-0.64, preferably .apprx.0.25-0.62, and more preferably .apprx.0.40-0.60, have the ability to make clear aq. fabric softener compns. contg. relatively high concns. of fabric softener actives having highly unsatd. hydrocarbon moieties or branched chains in 2 long-chain hydrophobic groups with specific cis/trans ratios and having long chain hydrocarbon groups with an iodine value .apprx.70-140 for the unsatd. groups corresponding to fatty acids with the same no. of carbons and the same configuration. The title compn. contains .ltorsim.40% solvents and 2-80% fabric softener actives, prepd. in the presence of chelating agent and/or antioxidant with reduced coloration and malodor. Premixes of the fabric softening actives, the principal solvents, and, optionally, other solvents are a preferred means of adding actives to complete formulations.

IT 187727-40-8, 3,4-Hexanediol, 2-methyl-  
(concd. aq. clear liq. fabric softening compn. with reduced malodor and coloration)  
RN 187727-40-8 ZCAPLUS  
CN 3,4-Hexanediol, 2-methyl- (9CI) (CA INDEX NAME)



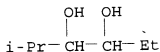


IT 187727-40-8, 3,4-Hexanediol, 2-methyl-  
(concd. aq. clear liq. fabric softening compn. with reduced  
malodor and coloration)

L28 ANSWER 4 OF 5 ZCAPLUS COPYRIGHT 2002 ACS  
1997:224021 Document No. 126:213656 Concentrated, water dispersible,  
stable, fabric softening compositions. Trinh, Toan; Tordil, Helen  
Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo  
Jean-Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton,  
James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark  
Robert; Vogel, Alice Marie; Rungta, Kamal Kumar; Sudarsana, Borra;  
Okamoto, Mitsuyo; et al. (Procter and Gamble Company, USA; Trinh,  
Toan; Tordil, Helen Bernardo; Wahl, Errol, Hoffman; Rinker,  
Jennifer, Lea; Demeyere, Hugo, Jean-Marie; Declercq, Marc, Johan;  
Gosselink, Eugene, Paul). PCT Int. Appl. WO 9703170 A1 19970130,  
111 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY,  
CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG,  
KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ,  
PL, PT, RO, RU, SD, SE, SG; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM,  
DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE.  
(English). CODEN: PIXXD2. APPLICATION: WO 1996-US11580 19960711.  
PRIORITY: US 1995-1057 19950711; US 1996-621019 19960322; US  
1996-638024 19960426.

AB The title aq., concd., stable, translucent, or preferably, clear,  
rinse added liq. fabric softening compns. which provide excellent  
water dispersibility in rinse water comprise a quaternary ammonium  
fabric softening active and a principal solvent of mainly diols or  
derivs. and mixts. thereof. To achieve the main object of excellent  
water dispersibility, the molar ratio of a principal solvent to a  
fabric softening active should be not less than 3, preferably from  
about 3.6-100, e.g., 1,2-hexanediol and dimethyldioleyleammonium  
chloride in 25.8:1 molar ratio, showing a homogeneous soln. in 50%  
diln. in cold water.

IT 187727-40-8  
(concd., water dispersible, stable, fabric softening compns.)  
RN 187727-40-8 ZCAPLUS  
CN 3,4-Hexanediol, 2-methyl- (9CI) (CA INDEX NAME)



IT 187727-40-8

(concd., water dispersible, stable, fabric softening compns.)

L28 ANSWER 5 OF 5 ZCAPLUS COPYRIGHT 2002 ACS

1997:215734 Document No. 126:200646 Solvents for concentrated, stable fabric softening composition. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Vogel, Alice Marie; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert (Procter and Gamble Company, USA; Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Vogel, Alice Marie; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; et al.). PCT Int. Appl. WO 9703169 A1 19970130, 277 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-US11556

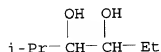
AB 19960711. PRIORITY: US 1995-1057 19950711; US 1996-621019 19960322. Principal solvents, esp. monools and diols, having a ClogP (calcd. logP, where P is the octanol-water partition coeff. of the substance) of 0.15-0.64, have the ability to make clear aq. fabric softener compns. contg. relatively high concns. of fabric softener actives having ester linkages in their long, hydrophobic chains. The fabric softener actives are either unsatd., or have intermediate length chains (.apprx.C12-14) and the principal solvents are used at levels of less than about 40 %. Other solvents may be present. Some of the principal solvents are novel compds. and/or novel mixts. Premixes of the fabric softening actives, the principal solvents, and, optionally, other solvents are useful in the prepn. of complete formulation by obviating/limiting the need for heating.

IT 187727-40-8

(solvents for concd., stable fabric softening compn.)

RN 187727-40-8 ZCAPLUS

CN 3,4-Hexanediol, 2-methyl- (9CI) (CA INDEX NAME)



IT 187727-40-8

(solvents for concd., stable fabric softening compn.)

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L29 ANSWER 1 OF 11 ZCAPLUS COPYRIGHT 2002 ACS

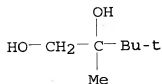
2002:271975 Document No. 136:296571 Concentrated, water dispersible, stable, fabric softening compositions. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert; Vogel, Alice Marie (The Procter & Gamble Company, USA). U.S. US 6369025 B1 20020409, 43 pp., Cont.-in-part of U.S. Ser. No. 638,024. (English). CODEN: USXXAM. APPLICATION: US 1998-983544 19980427. PRIORITY: US 1995-PV1057 19950711; US 1996-621019 19960322; US 1996-638024 19960426; WO 1996-US11580 19960711.

AB An aq., concd., stable, translucent, or preferably, clear, rinse added liq. fabric softening compn. provided excellent H2O dispersibility in rinse H2O, and comprises a fabric softening active and <40% principal solvent having a ClogP .apprx.0.15-0.64, and an asym. structure. Also, the compn. may contain <10% solvent selected from EtOH, isopropanol, propylene glycol, 1,3-propanediol, propylene carbonate, and mixts. In order to achieve excellent H2O dispersibility, the molar ratio of a principal solvent of a fabric softening active should be .gtoreq.3, preferably .apprx.3.6-100.

IT 100911-55-5 (concd., water dispersible, stable, fabric softening compns.)

RN 100911-55-5 ZCAPLUS

CN 1,2-Butanediol, 2,3,3-trimethyl- (6CI, 9CI) (CA INDEX NAME)

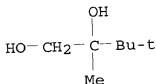


IT 100911-55-5 (concd., water dispersible, stable, fabric softening compns.)

L29 ANSWER 2 OF 11 ZCAPLUS COPYRIGHT 2002 ACS

2001:863494 Document No. 135:373284 Concentrated, stable clear fabric softening composition. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert; Vogel, Alice Marie (The Procter & Gamble Company, USA). U.S. US 6323172 B1 20011127, 126 pp., Cont.-in-part of U.S. Ser. No. 621,019, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1998-983542 19980925. PRIORITY: US 1996-621019 19960322; US 1996-620767 19960322; US 1996-620627 19960322; US 1996-620513 19960322; US 1996-621285 19960322; US 1996-621299 19960322; US 1996-621298 19960322; US 1996-620626 19960322; US 1996-620625 19960322; US 1996-620772 19960322; US 1996-621281 19960322; US 1996-620514

- 19960322; US 1996-620958 19960322; WO 1996-US11556 19960711.
- AB The title fabric softener contains 2-80% actives that are either unsatd., or have intermediate length chains (C12-14 ) e.g. N,N-di(cocoyloxyethyl)-N,N-dimethylammonium chloride, and principal solvents (.ltorsim.40%), esp. mono-ol and diol principal solvents, having a ClogP .apprx.0.15-0.64, preferably .apprx.0.25-0.62, and more preferably .apprx.0.40-0.60, which are not sym., optionally low mol. wt. water-sol. solvents, and optionally water-sol. Ca and/or Mg salts, and the balance water. An example clear liq. softener contained N,N-di(cocoyloxyethyl)-N,N-dimethylammonium chloride 27.5, EtOH 5.1, 1,2-hexanediol 16%, HCl 0.005, Kathon 3 ppm, and the balance water.
- IT 100911-55-5, 1,2-Butanediol, 2,3,3-trimethyl-  
(concn. aq. clear liq. fabric softening compn. contg.)
- RN 100911-55-5 ZCAPLUS
- CN 1,2-Butanediol, 2,3,3-trimethyl- (6CI, 9CI) (CA INDEX NAME)

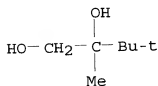


- IT 100911-55-5, 1,2-Butanediol, 2,3,3-trimethyl-  
(concn. aq. clear liq. fabric softening compn. contg.)
- L29 ANSWER 3 OF 11 ZCAPLUS COPYRIGHT 2002 ACS
- 1998:268582 Document No. 128:323167 Concentrated aqueous clear liquid fabric softening composition. Wahl, Errol Hoffman; Trinh, Toan; Oler, Chad James (Procter & Gamble Co., USA; Wahl, Errol Hoffman; Trinh, Toan; Oler, Chad James). PCT Int. Appl. WO 9817756 A1 19980430, 153 pp. DESIGNATED STATES: W: BR, CA, CN, JP, MX, US. (English). CODEN: PIXXD2. APPLICATION: WO 1997-US18932 19971021. PRIORITY: US 1996-28904 19961021.
- AB Principal solvents, esp. mono-ol and diol principal solvents, having a ClogP .apprx.0.15-0.64, preferably .apprx.0.25-0.62, and more preferably .apprx.0.40-0.60, have the ability to make clear aq. fabric softener compns. contg. relatively high concns. of fabric softener actives having highly unsatd. hydrocarbon moieties or branched chains in 2 long-chain hydrophobic groups with specific cis/trans ratios and having long chain hydrocarbon groups with an iodine value .apprx.70-140 for the unsatd. groups corresponding to fatty acids with the same no. of carbons and the same configuration. The title compn. contains .ltorsim.40% solvents and 2-80% fabric softener actives, prepd. in the presence of chelating agent and/or antioxidant with reduced coloration and malodor. Premixes of the fabric softening actives, the principal solvents, and, optionally, other solvents are a preferred means of adding actives to complete formulations.
- IT 100911-55-5, 1,2-Butanediol, 2,3,3-trimethyl-

(concd. aq. clear liq. fabric softening compn. with reduced  
malodor and coloration)

RN 100911-55-5 ZCAPLUS

CN 1,2-Butanediol, 2,3,3-trimethyl- (6CI, 9CI) (CA INDEX NAME)



IT 100911-55-5, 1,2-Butanediol, 2,3,3-trimethyl-  
(concd. aq. clear liq. fabric softening compn. with reduced  
malodor and coloration)

L29 ANSWER 4 OF 11 ZCAPLUS COPYRIGHT 2002 ACS

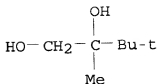
1997:224021 Document No. 126:213656 Concentrated, water dispersible,  
stable, fabric softening compositions. Trinh, Toan; Tordil, Helen  
Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo  
Jean-Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton,  
James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark  
Robert; Vogel, Alice Marie; Rungta, Kamal Kumar; Sudarsana, Borra;  
Okamoto, Mitsuyo; et al. (Procter and Gamble Company, USA; Trinh,  
Toan; Tordil, Helen Bernardo; Wahl, Errol, Hoffman; Rinker,  
Jennifer, Lea; Demeyere, Hugo, Jean-Marie; Declercq, Marc, Johan;  
Gosselink, Eugene, Paul). PCT Int. Appl. WO 9703170 A1 19970130,  
111 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY,  
CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG,  
KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ,  
PL, PT, RO, RU, SD, SE, SG; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM,  
DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE.  
(English). CODEN: PIXXD2. APPLICATION: WO 1996-US11580 19960711.  
PRIORITY: US 1995-1057 19950711; US 1996-621019 19960322; US  
1996-638024 19960426.

AB The title aq., concd., stable, translucent, or preferably, clear,  
rinse added liq. fabric softening compns. which provide excellent  
water dispersibility in rinse water comprise a quaternary ammonium  
fabric softening active and a principal solvent of mainly diols or  
derivs. and mixts. thereof. To achieve the main object of excellent  
water dispersibility, the molar ratio of a principal solvent to a  
fabric softening active should be not less than 3, preferably from  
about 3.6-100, e.g., 1,2-hexanediol and dimethyldioleyleammonium  
chloride in 25.8:1 molar ratio, showing a homogeneous soln. in 50%  
diln. in cold water.

IT 100911-55-5  
(concd., water dispersible, stable, fabric softening compns.)

RN 100911-55-5 ZCAPLUS

CN 1,2-Butanediol, 2,3,3-trimethyl- (6CI, 9CI) (CA INDEX NAME)



IT 100911-55-5

(concd., water dispersible, stable, fabric softening compns.)

L29 ANSWER 5 OF 11 ZCAPLUS COPYRIGHT 2002 ACS

1997:215734 Document No. 126:200646 Solvents for concentrated, stable fabric softening composition. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Vogel, Alice Marie; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert (Procter and Gamble Company, USA; Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Vogel, Alice Marie; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; et al.). PCT Int. Appl. WO 9703169 A1 19970130, 277 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-US11556 19960711. PRIORITY: US 1995-1057 19950711; US 1996-621019 19960322.

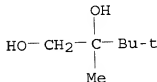
AB Principal solvents, esp. monools and diols, having a ClogP (calcd. logP, where P is the octanol-water partition coeff. of the substance) of 0.15-0.64, have the ability to make clear aq. fabric softener compns. contg. relatively high concns. of fabric softener actives having ester linkages in their long, hydrophobic chains. The fabric softener actives are either unsatd., or have intermediate length chains (.apprx.C12-14) and the principal solvents are used at levels of less than about 40 %. Other solvents may be present. Some of the principal solvents are novel compds. and/or novel mixts. Premixes of the fabric softening actives, the principal solvents, and, optionally, other solvents are useful in the prepn. of complete formulation by obviating/limiting the need for heating.

IT 100911-55-5

(solvents for concd., stable fabric softening compn.)

RN 100911-55-5 ZCAPLUS

CN 1,2-Butanediol, 2,3,3-trimethyl- (6CI, 9CI) (CA INDEX NAME)



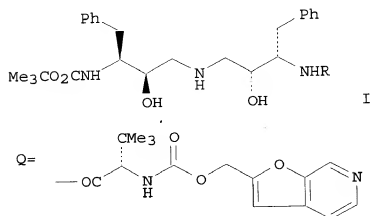
IT 100911-55-5

(solvents for concd., stable fabric softening compn.)

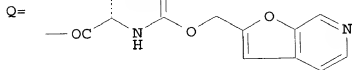
L29 ANSWER 6 OF 11 ZCAPLUS COPYRIGHT 2002 ACS

1996:637443 Document No. 125:329473 Preparation of  
 aminediol-containing peptide analogs as retroviral protease  
 inhibitors. Gordon, Eric M.; Barrish, Joel C.; Bisacchi, Gregory  
 S.; Sun, Chong-qing; Tino, Joseph A.; Vite, Gregory D.; Zahler,  
 Robert (E. R. Squibb & Sons, Inc., USA). U.S. US 5559256 A  
 19960924, 219 pp., Cont.-in-part of U.S. Ser. No. 927,027,  
 abandoned. (English). CODEN: USXXAM. APPLICATION: US 1993-79978  
 19930625. PRIORITY: US 1992-916916 19920720; US 1992-927027  
 19920806.

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*too recent*



AB Aa-E-NR8CHR9H(OH)CH<sub>2</sub>NHCH<sub>2</sub>CH(OH)CHR9NR8-E-Ab [Aa, Ab = H, alkyl, R<sub>3</sub>C(:Z), R<sub>3</sub>SO<sub>2</sub>, R<sub>3</sub>R<sub>4</sub>NSO<sub>2</sub>, R<sub>3</sub>R<sub>4</sub>NC(:Z), R<sub>3</sub>SC(:O), R<sub>5</sub>R<sub>6</sub>R<sub>7</sub>COC(:Z); E = a single bond or a peptide chain contg. 1 to 4 amino acids, the N-terminus of which is bonded to Aa or Ab; R<sub>3</sub>, R<sub>4</sub> = H, alkyl, aryl, carbocyclyl; R<sub>5</sub>, R<sub>6</sub>, R<sub>7</sub> = H, alkyl, aryl, carbocyclyl, fluorenyl, alkynyl, alkenyl; R<sub>5</sub>, R<sub>6</sub>, and R<sub>7</sub> may, independently, be joined together with the carbon atom to which they are bonded, to form a mono-, bi- or tricyclic carbocyclic ring system; R<sub>8</sub> = H, alkyl; R<sub>9</sub> = arylalkyl; Z = O, S; wherein: wherever they appear alone or as part of another group, unless otherwise indicated, the terms "alk." or "alkyl" denote a straight or branched chain satd. radical contg. 1 to 12 carbons in the normal chain, optionally substituted by one or more groups selected from (un)protected OH, oxo (with the proviso that the carbon bearing the oxo group is not adjacent to a heteroatom), CO<sub>2</sub>H, halo, alkoxy, aryloxy, alkoxycarbonyl, etc.] or salts thereof, which inhibit retroviral protease and are particularly useful in the treatment and/or prevention of HIV

infection (AIDS), are prepd. Thus, bis(3-amino-2-hydroxy-4-phenylbutyl)amine deriv. (I; R = H) was condensed with L-tert-leucine deriv. (HO-Q) using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride and HOBT in DMF/CH<sub>2</sub>CH<sub>2</sub> at 0.degree. to room temp. to give the title compd. I (R = Q). The latter compd. at 10 .mu.M in vitro inhibited 99% HIV protease and showed IC<sub>50</sub> of 0.012 .mu.M which was the concn. of drug that increased the formazan prodn. in CEM-SS cells infected with the RF strain of HIV to 50% of that produced by uninfected cells in the absence of drug.

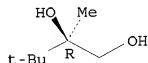
IT 162125-34-0P

(prepn. of aminediol-contg. peptide analogs as retroviral protease inhibitors for treatment of HIV infection (AIDS))

RN 162125-34-0 ZCAPLUS

CN 1,2-Butanediol, 2,3,3-trimethyl-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 162125-34-0P

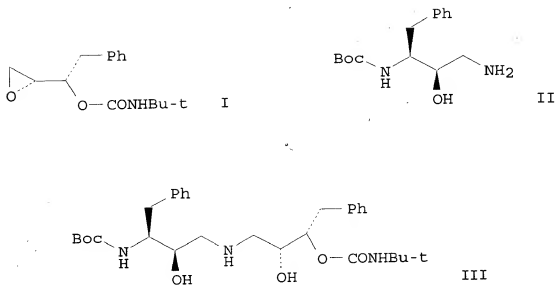
(prepn. of aminediol-contg. peptide analogs as retroviral protease inhibitors for treatment of HIV infection (AIDS))

L29 ANSWER 7 OF 11 ZCAPLUS COPYRIGHT 2002 ACS

1996:172219 Document No. 124:344117 Carbamate HIV protease inhibitors. Barrish, Joel C.; Spergel, Steven H. (Bristol-Myers Squibb Co., USA). U.S. US 5492910 A 19960220, 14 pp. (English). CODEN: USXXAM. APPLICATION: US 1994-341245 19941117.

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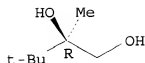




AB The invention discloses compds. A-E-NR5-CHR3-CH(OR1)-CH2-NH-CH2-CH(OR2)-CHR4-O2CNR6R7 including a pharmaceutically acceptable salt thereof wherein: R1 and R2 are independently selected from the group consisting of hydrogen, alkyl, substituted alkyl, alkylene-aryl, and alkylene-substituted aryl; R3 and R4 are independently selected from the group consisting of hydrogen, alkyl, substituted alkyl, cycloalkyl, aryl, substituted aryl, alkylene-aryl, alkylene-substituted aryl, alkylene-cycloalkyl, and alkylene-heterocyclo; R5 is hydrogen, alkyl, substituted alkyl, alkylene-aryl, or alkylene-substituted aryl; R6 and R7 are independently selected from the group consisting of hydrogen, alkyl, substituted alkyl, alkylene-aryl, and alkylene-substituted aryl and R6 and R7 taken together with the N-atom to which they are attached complete a heterocyclic ring of 5 to 7 atoms; A is H, alkyl, R8C(:Z), R8SO2, R6R7NSO2, R6R7NC(:Z), R8SC(:O), or R8R9R10COC(:Z); R8, R9, R10 are independently, e.g., H, alkyl, cycloalkyl, as HIV protease inhibitors. Thus, e.g., epoxide ring cleavage of tert-butylcarbamic acid, [S-(R\*,S\*)]-1-oxiranyl-2-phenylethyl ester (I, prepn. given) with [R-(R\*,S\*)]-[3-amino-2-hydroxy-1-(phenylmethyl)propyl]carbamic acid, tert-Bu ester (II, prepn. given) afforded [1S-[1R\*,2S\*(2S\*,3R\*)]]-3-[[[1,1-dimethylethyl]amino]carbonyloxy]-2-hydroxy-4-phenylbutyl]amino]-2-hydroxy-1-(phenylmethyl)propyl]carbamic acid, 1,1-dimethylethyl ester (III) which exhibited 98% inhibition of HIV protease at 10  $\mu$ M and an IC50 = 0.46  $\mu$ M for HIV (CEM cells).

IT 162125-34-OP  
(carbamate HIV protease inhibitors)  
RN 162125-34-0 ZCAPLUS  
CN 1,2-Butanediol, 2,3,3-trimethyl-, (R)- (9CI) (CA INDEX NAME)

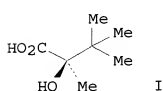
Absolute stereochemistry.



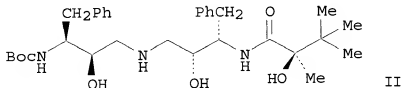
IT 162125-34-0P  
(carbamate HIV protease inhibitors)

L29 ANSWER 8 OF 11 ZCAPLUS COPYRIGHT 2002 ACS  
1996:19219 Document No. 124:202994 Synthesis and absolute configuration of (+)-2,3,3-trimethyl-2-hydroxybutanoic acid. Ahmad, Saleem; Spergel, Steven H.; Barrish, Joel C.; DiMarco, John; Gougoutas, Jack (Bristol-Myers Squibb Pharmaceutical Res. Institute, Princeton, NJ, 08543, USA). Tetrahedron: Asymmetry, 6(12), 2893-4 (English) 1995. CODEN: TASYE3. ISSN: 0957-4166. OTHER SOURCES: CASREACT 124:202994. Publisher: Elsevier.

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I



II

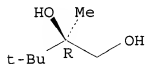
AB The abs. configuration of the title compd. (I), a key intermediate in the synthesis of the HIV-protease inhibitor II, has been confirmed as (R) by x-ray crystallog.

IT 162125-34-0P  
(synthesis and abs. configuration of HIV protease inhibitor intermediate trimethyl(hydroxy)butanoic acid)

RN 162125-34-0 ZCAPLUS

CN 1,2-Butanediol, 2,3,3-trimethyl-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

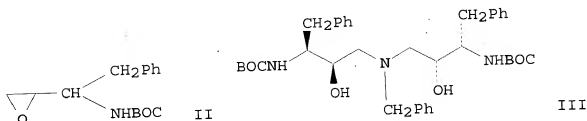
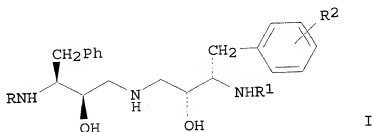


IT 162125-34-0P  
(synthesis and abs. configuration of HIV protease inhibitor intermediate trimethyl(hydroxy)butanoic acid)

L29 ANSWER 9 OF 11 ZCAPLUS COPYRIGHT 2002 ACS

1995:511385 Document No. 122:290438 Preparation of diphenyl-substituted amino alcohols as protease inhibitors. Gordon, Eric M.; Barrish, Joel C.; Bisacchi, Gregory S.; Sun, Chong Qing; Tino, Joseph A.; Vite, Gregory D.; Zahler, Robert (Squibb, E. R., and Sons, Inc., USA). Eur. Pat. Appl. EP 580402 A2 19940126, 393 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE. (English). CODEN: EPXXDW. APPLICATION: EP 1993-305691 19930720. PRIORITY: US 1992-916916 19920720; US 1992-927027 19920806; US 1993-79978 19930625.

GI



AB Novel amino alcs. [I; R, R1 = protecting group, substituent; R2 = H, substituent], useful in inhibiting retroviral protease, particularly useful in the treatment and/or prevention of HIV infection (AIDS), are prep'd. A mixt. of 2:1 II/PhCH2NH2 was heated at 105-108.degree. under Ar to give 56% III, which was refluxed over 20% Pd(OH)2/C in EtOH-cyclohexene to give 69% I (R = R1 = Boc, R2 = H), which showed 100% inhibition of HIV protease at 10 .mu.M and IC50 of 0.09 .mu.M against HIV CEM cells.

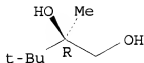
IT 162125-34-0P

(prepn. of diphenyl-substituted amino alcs. as protease inhibitors)

RN 162125-34-0 ZCAPLUS

CN 1,2-Butanediol, 2,3,3-trimethyl-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 162125-34-0P

(prepn. of diphenyl-substituted amino alcs. as protease inhibitors)

L29 ANSWER 10 OF 11 ZCAPLUS COPYRIGHT 2002 ACS

1995:18086 Document No. 122:234164 The rabbit liver microsomal biotransformation of 1,1-dialkylethylenes: enantioface selection of epoxidation and enantioselectivity of epoxide hydrolysis. Bellucci, Giuseppe; Chiappe, Cinzia; Cordoni, Antonio; Marioni, Franco (Dep. Bioorg. Chem., Univ. Pisa, Pisa, Italy). Chirality, 6(3), 207-12 (English) 1994. CODEN: CHRLP. ISSN: 0899-0042.

AB The rabbit liver microsomal biotransformation of .alpha.-methylstyrene, 2-methyl-1-hexene, 2,4,4-trimethyl-1-pentene, and 2,3,3-trimethyl-1-butene has been investigated with the aim at establishing the enantioface selection of the cytochrome P 450-promoted epoxidn. of the double bond and the enantioselectivity of microsomal epoxide hydrolase (mEH)-catalyzed hydrolysis of the resulting epoxides. GLC on a Chiraldex G-TA (ASTEC) column was used to det. the enantiomeric compn. of the products. The epoxides first produced in incubations carried out in the presence of an NADPH regenerating system were not detected, being rapidly hydrolyzed by mEH to diols. A comparison of these results with those previously obtained for linear and branched chain alkyl monosubstituted oxiranes shows that the introduction of the second alkyl substituent suppresses the selectivity of the mEH reaction of the latter and reverses that of the former substrates.

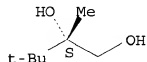
IT 116199-30-5P 162125-34-0P

(rabbit liver microsomal biotransformation of dialkylethylenes: enantioface selection of epoxidn. and enantioselectivity of epoxide hydrolysis)

RN 116199-30-5 ZCAPLUS

CN 1,2-Butanediol, 2,3,3-trimethyl-, (S)- (9CI) (CA INDEX NAME)

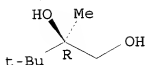
Absolute stereochemistry.



RN 162125-34-0 ZCAPLUS

CN 1,2-Butanediol, 2,3,3-trimethyl-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 116199-30-5P 162125-34-0P

(rabbit liver microsomal biotransformation of dialkylethylenes:  
enantioface selection of epoxidn. and enantioselectivity of  
epoxide hydrolysis)

L29 ANSWER 11 OF 11 ZCAPLUS COPYRIGHT 2002 ACS

1988:610281 Document No. 109:210281 The configuration of  
(-)-2,3,3-trimethyl-2-hydroxybutanoic acid, Me<sub>3</sub>CCMe(OH)CO<sub>2</sub>H,  
(-)-3,3,4-trimethyl-3-hydroxy-1-pentyne, and (-)-3-tert-butyl-3-  
methyl-1-chloroallene. Eliel, Ernest L.; Lynch, Joseph E. (William  
R. Kenan, Jr. Lab. Chem., Univ. North Carolina, Chapel Hill, NC,  
27514, USA). Tetrahedron Lett., 28(41), 4813-16 (English) 1987.  
CODEN: TELEAY. ISSN: 0040-4039. OTHER SOURCES: CASREACT  
109:210281.

AB The configurations of the title compds. are reassigned, based on  
stereoselective syntheses of the hydroxy acid and corresponding  
glycol and application of Cram's, Prelog's and Sharpless' rules.

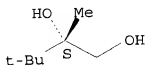
IT 116199-30-5P

(prepn. and abs. configuration of)

RN 116199-30-5 ZCAPLUS

CN 1,2-Butanediol, 2,3,3-trimethyl-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 116199-30-5P

(prepn. and abs. configuration of)

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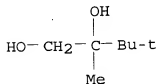
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substance identification. Title keywords, authors, patent

assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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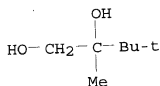
L23 ANSWER 1 OF 3 CAOLD COPYRIGHT 2002 ACS  
 AN CA51:17727e CAOLD  
 TI rearrangement of .alpha..beta.-unsatd. alcs. to satd. aldehydes and ketones - (II) course of the rearrangement  
 AU Green, Maurice B.; Hickinbottom, W. J.  
 IT 513-42-8 4364-51-6 4435-54-5 26903-66-2 39497-64-8  
 41051-72-3 50965-90-7 56255-50-6 66553-15-9 81280-12-8  
 100911-55-5  
 IT 100911-55-5  
 RN 100911-55-5 CAOLD  
 CN 1,2-Butanediol, 2,3,3-trimethyl- (6CI, 9CI) (CA INDEX NAME)



L23 ANSWER 2 OF 3 CAOLD COPYRIGHT 2002 ACS  
 AN CA51:17725i CAOLD  
 TI rearrangement of .alpha..beta.-unsatd. alcs. to satd. aldehydes and ketones - (I) prepn. of .alpha..beta.-unsatd. alcs. and 1,2-diols and their prototropic change  
 AU Green, Maurice B.; Hickinbottom, W. J.  
 IT 77-70-3 80-55-7 96-17-3 97-96-1 123-05-7  
 123-15-9 497-03-0 513-42-8 592-64-3 617-67-4 623-36-9  
 922-63-4 925-54-2 994-26-3 1070-13-9 1070-43-5 1070-66-2  
 1617-38-5 2109-98-0 2177-38-0 2747-54-8 3491-57-4  
 4364-51-6 4417-80-5 4435-54-5 4798-58-7 5582-86-5  
 5665-82-7 6038-09-1 6137-03-7 6137-14-0 6137-15-1  
 7379-12-6 7511-26-4 10473-13-9 17042-16-9 17408-48-9  
 17773-74-9 19310-95-3 19780-25-7 20667-04-3 20754-04-5  
 21101-97-3 21101-98-4 22092-54-2 24580-44-7 26903-66-2  
 32493-36-0 33861-38-0 33861-40-4 39497-64-8 40239-42-7  
 41051-72-3 50468-22-9 50639-00-4 50965-90-7 53516-67-9  
 53555-58-1 56255-50-6 57003-66-4 63818-27-9 66553-15-9  
 66553-16-0 69060-18-0 72486-21-6 84065-11-2 89856-15-5  
 93667-58-4 98278-60-5 98487-55-9 98560-72-6 98955-05-6

98955-06-7 98955-64-7 100387-56-2 100869-08-7 100911-55-5  
 101084-24-6 101084-25-7 101257-00-5 102369-71-1 102370-20-7  
 102438-74-4 102450-27-1 102450-28-2 102450-30-6 102877-66-7  
 102877-72-5 103985-90-6 103985-91-7 106594-50-7 117500-54-6  
 117713-46-9  
 100911-55-5

IT 100911-55-5 CAOLD  
 RN 1,2-Butanediol, 2,3,3-trimethyl- (6CI, 9CI) (CA INDEX NAME)  
 CN

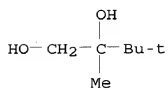


L23 ANSWER 3 OF 3 CAOLD COPYRIGHT 2002 ACS

AN CA51:2707c CAOLD  
 TI velocity of cleavage with Pb tetraacetate in relation to the  
 constitution and configuration of the glycol - (III)  
 AU Criegee, Rudolf; Hoeger, E.; Huber, G.; Kruck, P.; Marktscheffel,  
 F.; Schellenberger, H.

IT 93-56-1 464-72-2 492-70-6 943-96-4 1069-23-4  
 1117-86-8 1119-87-5 1124-96-5 1636-34-6 2888-11-1  
 2955-63-7 2955-64-8 3710-31-4 4065-92-3 4486-59-3  
 5181-75-9 5396-58-7 5557-31-3 5607-45-4 6217-22-7  
 6296-92-0 6730-95-6 6931-71-1 6948-59-0 6970-72-5  
 7251-51-6 13505-34-5 13603-63-9 14619-90-0 14619-92-2  
 15584-48-2 15679-25-1 15753-47-6 15810-14-7 15870-10-7  
 15962-87-5 16162-34-8 16177-37-0 16343-75-2 18021-17-5  
 22607-10-9 24017-95-6 25061-77-2 27956-09-8 28509-09-3  
 28622-70-0 33969-55-0 34780-00-2 37399-02-3 40459-97-0  
 41248-13-9 42082-92-8 49578-06-5 50468-22-9 55489-05-9  
 56363-86-1 57132-07-7 59562-82-2 60566-02-1 64484-85-1  
 65213-66-3 65678-03-7 65834-10-8 66553-16-0 69180-46-7  
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 90676-29-2 91635-53-9 94465-37-9 94616-99-6 98560-25-9  
 98880-19-4 98955-30-7 99115-05-6 99115-92-1 99182-91-9  
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 103153-96-4 103155-81-3 103161-65-5 103277-77-6 103281-30-7  
 103394-01-0 103862-24-4 103985-44-0 104622-96-0 105901-35-7  
 109251-16-3 109253-89-6 109939-30-2 115001-35-9 115122-45-7  
 115210-52-1 116027-68-0 116570-16-2 128927-39-9  
 100911-55-5

IT 100911-55-5 CAOLD  
 RN 1,2-Butanediol, 2,3,3-trimethyl- (6CI, 9CI) (CA INDEX NAME)  
 CN





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L30 ANSWER 1 OF 7 ZCAPLUS COPYRIGHT 2002 ACS

2002:271975 Document No. 136:296571 Concentrated, water dispersible, stable, fabric softening compositions. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert; Vogel, Alice Marie (The Procter & Gamble Company, USA). U.S. US 6369025 B1 20020409, 43 pp., Cont.-in-part of U.S. Ser. No. 638,024. (English). CODEN: USXXAM. APPLICATION: US 1998-983544 19980427. PRIORITY: US 1995-PV1057 19950711; US 1996-621019 19960322; US 1996-638024 19960426; WO 1996-US11580 19960711.

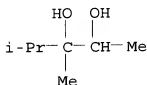
AB An aq., concd., stable, translucent, or preferably, clear, rinse added liq. fabric softening compn. provided excellent H2O dispersibility in rinse H2O, and comprises a fabric softening active and <40% principal solvent having a ClogP .apprx.0.15-0.64, and an asym. structure. Also, the compn. may contain <10% solvent selected from EtOH, isopropanol, propylene glycol, 1,3-propanediol, propylene carbonate, and mixts. In order to achieve excellent H2O dispersibility, the molar ratio of a principal solvent of a fabric softening active should be .gtoreq.3, preferably .apprx.3.6-100.

IT 187727-33-9

(concd., water dispersible, stable, fabric softening compns.)

RN 187727-33-9 ZCAPLUS

CN 2,3-Pentanediol, 3,4-dimethyl- (9CI) (CA INDEX NAME)



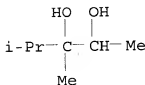
IT 187727-33-9

(concd., water dispersible, stable, fabric softening compns.)

L30 ANSWER 2 OF 7 ZCAPLUS COPYRIGHT 2002 ACS

2001:863494 Document No. 135:373284 Concentrated, stable clear fabric softening composition. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert; Vogel, Alice Marie (The Procter & Gamble Company, USA). U.S. US 6323172 B1 20011127, 126 pp., Cont.-in-part of U.S. Ser. No. 621,019, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1998-983542 19980925. PRIORITY: US 1996-621019 19960322; US 1996-620767 19960322; US 1996-620627 19960322; US 1996-620513 19960322; US 1996-621285 19960322; US 1996-621299 19960322; US 1996-621298 19960322; US 1996-620626 19960322; US 1996-620625 19960322; US 1996-620772 19960322; US 1996-621281 19960322; US 1996-620514

- 19960322; US 1996-620958 19960322; WO 1996-US11556 19960711.
- AB The title fabric softener contains 2-80% actives that are either unsatd., or have intermediate length chains (C12-14 ) e.g. N,N-di(cocoyloxyethyl)-N,N-dimethylammonium chloride, and principal solvents (.ltorsim.40%), esp. mono-ol and diol principal solvents, having a ClogP .apprx.0.15-0.64, preferably .apprx.0.25-0.62, and more preferably .apprx.0.40-0.60, which are not sym., optionally low mol. wt. water-sol. solvents, and optionally water-sol. Ca and/or Mg salts, and the balance water. An example clear liq. softener contained N,N-di(cocoyloxyethyl)-N,N-dimethylammonium chloride 27.5, EtOH 5.1, 1,2-hexanediol 16%, HCl 0.005, Kathon 3 ppm, and the balance water.
- IT 187727-33-9, 2,3-Pentanediol, 3,4-dimethyl-  
(concn. aq. clear liq. fabric softening compn. contg.)
- RN 187727-33-9 ZCAPLUS
- CN 2,3-Pentanediol, 3,4-dimethyl- (9CI) (CA INDEX NAME)

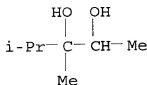


- IT 187727-33-9, 2,3-Pentanediol, 3,4-dimethyl-  
(concn. aq. clear liq. fabric softening compn. contg.)
- L30 ANSWER 3 OF 7 ZCAPLUS COPYRIGHT 2002 ACS
- 1998:268582 Document No. 128:323167 Concentrated aqueous clear liquid fabric softening composition. Wahl, Errol Hoffman; Trinh, Toan; Oler, Chad James (Procter & Gamble Co., USA; Wahl, Errol Hoffman; Trinh, Toan; Oler, Chad James). PCT Int. Appl. WO 9817756 A1 19980430, 153 pp. DESIGNATED STATES: W: BR, CA, CN, JP, MX, US. (English). CODEN: PIXXD2. APPLICATION: WO 1997-US18932 19971021. PRIORITY: US 1996-28904 19961021.
- AB Principal solvents, esp. mono-ol and diol principal solvents, having a ClogP .apprx.0.15-0.64, preferably .apprx.0.25-0.62, and more preferably .apprx.0.40-0.60, have the ability to make clear aq. fabric softener compns. contg. relatively high concns. of fabric softener actives having highly unsatd. hydrocarbon moieties or branched chains in 2 long-chain hydrophobic groups with specific cis/trans ratios and having long chain hydrocarbon groups with an iodine value .apprx.70-140 for the unsatd. groups corresponding to fatty acids with the same no. of carbons and the same configuration. The title compn. contains .ltorsim.40% solvents and 2-80% fabric softener actives, prepd. in the presence of chelating agent and/or antioxidant with reduced coloration and malodor. Premixes of the fabric softening actives, the principal solvents, and, optionally, other solvents are a preferred means of adding actives to complete formulations.
- IT 187727-33-9, 2,3-Pentanediol, 3,4-dimethyl-

(concd. aq. clear liq. fabric softening compn. with reduced  
malodor and coloration)

RN 187727-33-9 ZCAPLUS

CN 2,3-Pentanediol, 3,4-dimethyl- (9CI) (CA INDEX NAME)



IT 187727-33-9, 2,3-Pentanediol, 3,4-dimethyl-  
(concd. aq. clear liq. fabric softening compn. with reduced  
malodor and coloration)

L30 ANSWER 4 OF 7 ZCAPLUS COPYRIGHT 2002 ACS

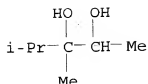
1997:224021 Document No. 126:213656 Concentrated, water dispersible,  
stable, fabric softening compositions. Trinh, Toan; Tordil, Helen  
Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Demeyere, Hugo  
Jean-Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton,  
James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark  
Robert; Vogel, Alice Marie; Rungta, Kamal Kumar; Sudarsana, Borra;  
Okamoto, Mitsuyo; et al. (Procter and Gamble Company, USA; Trinh,  
Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker,  
Jennifer, Lea; Demeyere, Hugo, Jean-Marie; Declercq, Marc, Johan;  
Gosselink, Eugene, Paul). PCT Int. Appl. WO 9703170 A1 19970130,  
111 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY,  
CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG,  
KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ,  
PL, PT, RO, RU, SD, SE, SG; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM,  
DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE.  
(English). CODEN: PIXXD2. APPLICATION: WO 1996-US11580 19960711.  
PRIORITY: US 1995-1057 19950711; US 1996-621019 19960322; US  
1996-638024 19960426.

AB The title aq., concd., stable, translucent, or preferably, clear,  
rinse adduct liq. fabric softening compns. which provide excellent  
water dispersibility in rinse water comprise a quaternary ammonium  
fabric softening active and a principal solvent of mainly diols or  
derivs. and mixts. thereof. To achieve the main object of excellent  
water dispersibility, the molar ratio of a principal solvent to a  
fabric softening active should be not less than 3, preferably from  
about 3.6-100, e.g., 1,2-hexanediol and dimethyldioleammonium  
chloride in 25.8:1 molar ratio, showing a homogeneous soln. in 50%  
diln. in cold water.

IT 187727-33-9  
(concd., water dispersible, stable, fabric softening compns.)

RN 187727-33-9 ZCAPLUS

CN 2,3-Pentanediol, 3,4-dimethyl- (9CI) (CA INDEX NAME)



IT 187727-33-9

(concd., water dispersible, stable, fabric softening compns.)

L30 ANSWER 5 OF 7 ZCAPLUS COPYRIGHT 2002 ACS

1997:215734 Document No. 126:200646 Solvents for concentrated, stable fabric softening composition. Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Vogel, Alice Marie; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; Letton, James Carey; Back, Deborah Jean; Severns, John Cort; Sivik, Mark Robert (Procter and Gamble Company, USA; Trinh, Toan; Tordil, Helen Bernardo; Wahl, Errol Hoffman; Rinker, Jennifer Lea; Vogel, Alice Marie; Demeyere, Hugo Jean Marie; Declercq, Marc Johan; Gosselink, Eugene Paul; et al.). PCT Int. Appl. WO 9703169 A1 19970130, 277 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-US11556

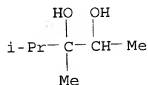
AB 19960711. PRIORITY: US 1995-1057 19950711; US 1996-621019 19960322. Principal solvents, esp. monools and diols, having a ClogP (calcd. logP, where P is the octanol-water partition coeff. of the substance) of 0.15-0.64, have the ability to make clear aq. fabric softener compns. contg. relatively high concns. of fabric softener actives having ester linkages in their long, hydrophobic chains. The fabric softener actives are either unsatd., or have intermediate length chains (.apprx.C12-14) and the principal solvents are used at levels of less than about 40 %. Other solvents may be present. Some of the principal solvents are novel compds. and/or novel mixts. Premixes of the fabric softening actives, the principal solvents, and, optionally, other solvents are useful in the prepn. of complete formulation by obviating/limiting the need for heating.

IT 187727-33-9

(solvents for concd., stable fabric softening compn.)

RN 187727-33-9 ZCAPLUS

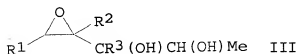
CN 2,3-Pentanediol, 3,4-dimethyl- (9CI) (CA INDEX NAME)



IT 187727-33-9  
(solvents for concd., stable fabric softening compn.)

L30 ANSWER 6 OF 7 ZCAPLUS COPYRIGHT 2002 ACS  
1993:560002 Document No. 119:160002 Direct epoxy hydroxylation of hydroperoxy homoallylic alcohols: multidentate oxygen donor and oxygen acceptor substrates in titanium(IV)-catalyzed epoxidations. Adam, Waldemar; Nestler, Bernd (Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, D-8700, Germany). Journal of the American Chemical Society, 115(16), 7226-31 (English) 1993. CODEN: JACSAT. ISSN: 0002-7863.

GI



AB The hydroperoxy homoallylic alcs. (R\*,S\*)-CH<sub>2</sub>:CMeCH(OOH)CH(OH)Me and (S\*,S\*)-R<sub>1</sub>CH:CR<sub>2</sub>CR<sub>3</sub>(OOH)CH(OH)Me (I; R<sub>1</sub> = H, Bu; R<sub>2</sub>, R<sub>3</sub> = H, Me), readily available through the photooxygenation of chiral allylic alcs. R<sub>1</sub>CH<sub>2</sub>CR<sub>2</sub>:CR<sub>3</sub>CH(OH)Me (II), were converted to epoxy diols (III) under the catalytic action of Ti(OCHMe<sub>2</sub>)<sub>4</sub>. In these epoxy hydroxylations, the hydroperoxides play a double role as oxygen atom donor and, in the form of the in situ generated corresponding unsatd. diols (IV), as substrate for oxygen transfer. Compared to Ti(IV)-catalyzed epoxidns. of unsatd. diols by tert-BuOOH, the advantage of this approach is that a large rate enhancement is obtained. Moreover, with the exception of I (R<sub>1</sub> = R<sub>2</sub> = H, R<sub>3</sub> = Me), all reactions proceeded with unusually high diastereoselectivity. These results are rationalized in terms of the ability of the hydroxy-functionalized hydroperoxides (oxygen atom donors) as well as IV (oxygen atom acceptors) to chelate to the titanium metal in the catalytically operating template. For some IV bidentate binding is feasible, while for other IV this is difficult due to unfavorable steric interactions. Important for synthetic applications is the fact that II can be directly converted to III in a one-pot, two-step procedure simply by adding catalytic amts. of Ti(OCHMe<sub>2</sub>)<sub>4</sub> to a photooxygenated soln. of II.

IT 150129-17-2  
(reaction of, with titanium tetra-tert-butoxide)

RN 150129-17-2 ZCAPLUS

IT 150129-17-2  
(reaction of, with titanium tetra-tert-butoxide)

L30 ANSWER 7 OF 7 ZCAPLUS COPYRIGHT 2002 ACS  
1973:97026 Document No. 78:97026 Stereoselectivity in the reduction of aliphatic .alpha.-ketols with aluminum hydride reagents. Katzenellenbogen, John A.; Bowlus, Stephen B. (Dep. Chem., Univ.

Illinois, Urbana, Ill., USA). J. Org. Chem., 38(4), 627-32  
(English) 1973. CODEN: JOCEAH.

AB Redn. of 6 .alpha.-ketols with different patterns of substitution and size of substituents was investigated using 7 Al hydride reagents. The ratio of diastereomeric diols produced was detd. by 220 MHz NMR anal. In each case the predominant diol was the one predicted by Cram's cyclic model. The degree of stereoselectivity correlates well with .alpha.-ketol structure with only 1 reagent (triisobutylaluminum). With the other (agglomerated) reagents, selectivity is related only in an irregular manner to .alpha.-ketol structure.

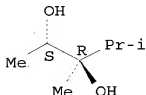
IT 37164-04-8P 37164-05-9P

(prepn. and configuration of, NMR in relation to)

RN 37164-04-8 ZCAPLUS

CN 2,3-Pentanediol, 3,4-dimethyl-, (R\*,S\*)- (9CI) (CA INDEX NAME)

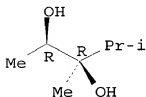
Relative stereochemistry.



RN 37164-05-9 ZCAPLUS

CN 2,3-Pentanediol, 3,4-dimethyl-, (R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 37164-04-8P 37164-05-9P

(prepn. and configuration of, NMR in relation to)